

REGISTRATION: 07:00-18:00

Opening Ceremony

9:00 - 9:30

LIFE SCIENCES INSTITUTE 2

- 9:00 **Adam Hitchcock** Welcome to VUVX2010
 9:10 **John Hepburn** Welcome from UBC
 9:20 **Josef Hormes** Welcome from CLS
 9:25 **Stephen Urquhart** Organizational details

2PL Novel materials

Chair: Adam Hitchcock

9:30 - 10:10

LIFE SCIENCES INSTITUTE 2

2PL1 **Alessandra Lanzara** (plenary)

- 9:30 Many body interactions in freestanding and epitaxial graphene

Coffee

10:10 - 10:40

2A High energy photoelectron spectroscopy

Chair: Amina Taleb-Ibrahimi

10:40 - 12:30

LIFE SCIENCES INSTITUTE 2

2A1 **Yasutaka Takata** (invited)

- 10:40 Hard X-ray photoelectron spectroscopy

2A2 **Gerhard Fecher**

- 11:10 Hard X-ray photoelectron spectroscopy (HAXPES) with variable photon polarization: linear and circular dichroism

2A3 **Giancarlo Panaccione**

- 11:30 Depth dependence of itinerant character in $\text{Sr}_3\text{Ru}_{1-x}\text{Mn}_x\text{O}_7$; evolution upon Mn doping

2A4 **Marcus Bär**

- 11:50 Investigation of the buried silicon/zinc oxide interface by soft X-ray emission and hard X-ray photoelectron spectroscopy

2A5 **Yves Joly**

- 12:10 X-ray absorption near edge structure and resonant X-ray diffraction simulations applied to the study of oxides

2B Atoms and Molecules (1)

Chair: Paul Morin

10:40 - 12:30

FOREST SCIENCES 1005

2B1 **Catalin Miron** (invited)

- 10:40 Decay dynamics and nuclear motion of core-excited species probed by high resolution soft X-ray electron spectroscopy

2B2 **Itaru Higuchi**

- 11:10 Interatomic Coulombic decay and electron transfer mediated decay after triple ionization of Ar dimer

2B3 **Michael Chini**

- 11:30 Attosecond-resolved autoionization in Argon

2B4 **Burkhard Langer**

- 11:50 Photoinduced localization and decoherence in inversion symmetric molecules

2B5 **Christian Alcaraz**

- 12:10 VUV threshold photoionization of hydrocarbon radicals

Lunch

12:30 - 14:00

2C Scattering and X-ray emission

Chair: Alex Moewes

14:00 - 16:10

LIFE SCIENCES INSTITUTE 2

2C1 **Giacomo Ghiringhelli** (invited)

- 14:00 Momentum dependent excitations in cuprates studied by high resolution RIXS

2C2 **Joanna Hozzowska**

- 14:30 First observation of two-electron one-photon transitions in single-photon impact

2C3 **Akio Kotani**

- 14:50 A new method of directly determining the core-hole effect in the Ce L_3 XAS of mixed valence Ce compounds

2C4 **Regan Wilks**

- 15:10 Band-mapping and above-valence emission in Si photovoltaic materials studied using RIXS

2C5 **Thorsten Schmitt**

- 15:30 Dispersion of two-spinon and collective orbital excitations in Sr_2CuO_3 investigated by resonant inelastic X-ray scattering

2C6 **Maurits Haverkort**

- 15:50 Coexistence of bound and virtual-bound states in shallow-core to valence spectroscopies

2D Materials & Surface Science

Chair: Dominique Chandesris

14:00 - 16:10

FOREST SCIENCES 1005

2D1 **John Tse** (invited)

- 14:00 Characterization of materials at high pressure with synchrotron radiation

2D2 **Luca Petaccia**

- 14:30 Electronic structure of strongly correlated materials: novel spectroscopic approaches from the VUV to the hard X-rays

2D3 **Yosuke Nakashima**

- 14:50 Three-dimensional Fermi-surface mapping of BaFe_2As_2 using low-energy angle-resolved photoemission spectroscopy

2D4 **Moritz Speckmann**

- 15:10 Facets, mazes, slabs, and nanowires: silver-mediated germanium growth on silicon surfaces

2D5 **Olga Molodtsova**

- 15:30 Formation of ferromagnetic metal top contacts on an organic semiconductor in soft landing conditions: evidence for a sharp, mainly nonreactive interface

2D6 **Liang Cao**

- 15:50 Molecular orientation and charge transfer dynamics studies of PTCDAs on Au(111)

POSTER SESSION 2P

Chair: Yongfeng Hu

EAST AND WEST ATRIA, LIFE SCIENCES CENTRE

16:10 - 18:00

2PL1

Many body interactions in freestanding and epitaxial graphene

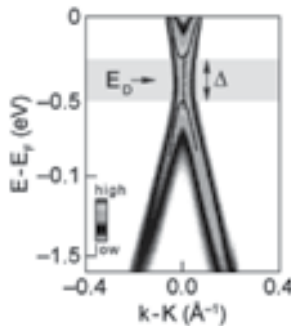
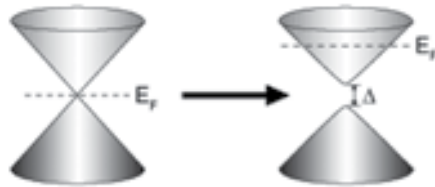
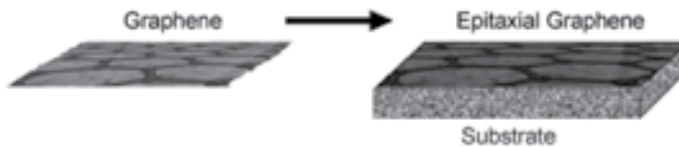
Alessandra Lanzara^{1,2}

¹ University California, Berkeley, Berkeley, CA, United States.

² Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States.

In this talk I will present a summary of our experimental work in the emerging field of graphene using high resolution angle resolved photoemission spectroscopy. I'll present our study of many body interactions and how they evolve away from half filling and provide compelling evidence of the departure from a Fermi liquid picture. Finally, by comparing our results on epitaxial and freestanding graphene I'll discuss how the substrate can affect many body interactions, screening and the general electronic structure of Dirac fermions. The evolution of many body interaction with doping, defects and quantum confinement are also discussed. The implications of our study on the properties of Dirac materials and their potential role for applications are discussed.

Right: In graphene's electronic band structure, the conduction and valence bands just meet at the Fermi energy (EF), so there is no band gap.



Left: When a graphene layer is grown on a silicon carbide substrate, symmetry is broken which opens a gap [Δ] around the Dirac energy [ED], between the valence and conduction bands, as shown in the ARPES band map (lower right)



Alessandra Lanzara received her PhD in Physics from the University of Rome "La Sapienza" in 1999. From 1999 to 2002 she worked as a post-doc at Stanford University. In 2002 she joined the Physics Department of the University of California, Berkeley as an Assistant Professor and became Associate Professor in 2006. She also has a joint faculty appointment in the Materials Sciences Division of the Lawrence Berkeley National Laboratory. Prof. Lanzara's work has received several prestigious prizes such as the MacMillan Award (2003), the Shirley Award (2007) and the Marie Goeppert Mayer award from the American Physical Society (2010). In 2008 she was elected Fellow of the American Physical Society. Prof. Lanzara has authored more than 100 papers in high profile scientific journals and several scientific and general media outlets have featured her research.

Her main research interests lie on the frontier aspects of condensed matter physics, motivated by the search for new states of matter with the main focus being on high temperature superconductivity and Dirac materials such as graphene and topological insulators. She is also pushing the frontier of photoemission spectroscopy to the time and spin realm, with the development of a novel concept of electron energy analyzer for spin detection.

2A1 (Invited)

Hard X-ray photoelectron spectroscopy

Y Takata¹¹RIKEN SPring-8 Center, Sayo-cho, Sayo-gun, Hyogo, Japan

Photoelectron Spectroscopy (PES) is a powerful method to investigate electronic structure of materials. However, conventional vacuum ultraviolet (VUV) and soft X-ray (SX) PES is surface sensitive because of the short inelastic-mean-free-paths of photoelectrons. In order to realize bulk-sensitive or surface-insensitive PES, hard X-ray PES (HAXPES) using high-brilliance synchrotron radiation has been developed. A combination of X-ray optics and an electron energy analyzer dedicated for HAXPES achieved the total instrumental energy resolution of 55 meV (FWHM) at 7.94 keV at BL29XU in SPring-8 [1-3]. Large probing depth of high energy photoelectrons enables us to probe intrinsic bulk electronic structure. New functional materials such as MBE-grown thin layers are accessible even after structural, electric and magnetic characterization by other techniques in air or low vacuum. We will show the performance of our apparatus and demonstrate the importance of this method in the form of results on various materials[4-10]. We will also report the recoil effect of high energy photoelectrons from light elements[11].

[1] K. Kobayashi et al., APL, **83**, 1005 (2003), [2] T. Ishikawa et al., NIM, **A 547**, 42 (2005), [3] Y. Takata et al., NIM, **A 547**, 50 (2005), [4] A. Chainani et al., PRB **69**, R180508 (2004), [5] K. Horiba et al., PRL **93**, 236401 (2004). [6] H. Sato et al., PRL **93**, 246404 (2004), [7] M. Taguchi et al., PRL **95**, 177002 (2005), [8] M. Matsunami et al., PRB **77**, 165126 (2008). [9] M. Takizawa et al., PRL **102**, 236401 (2009), [10] M. Taguchi et al., PRL **104**, 106401 (2010). [11] Y. Takata et al., PRB **75**, 233404 (2007), PRL **101**, 137601 (2008).

2A2

Hard X-ray photoelectron spectroscopy (HAXPES) with variable photon polarization: linear and circular dichroism

G H Fecher,¹ G Stryganyuk,¹ X Kozina,¹ S Ouardi,¹ B Balke,¹ C Felser,¹ E Ikenaga,² K Kobayashi³¹Johannes Gutenberg - University, Mainz, Germany; ²Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan;³National Institute for Materials Science, SPring-8, Hyogo, Japan

We report on the first photoemission experiments using hard X-rays (8 keV) with variable polarization for excitation. The polarization of the hard X-rays is changed using an in-vacuum diamond phase retarder. The initial linear p polarization can be changed to linear s or circular (σ^+ , σ^-). The variation of the polarization enables to measure linear as well as circular dichroism in the angular distribution of the photoelectrons. The high bulk sensitivity of HAXPES is suitable to determine the magnetism in magnetic multilayers making use of the magnetic dichroism from core-levels and valence band. Linear dichroism experiments were performed on NiTiSn and NiMnSb bulk samples. The change from p to s polarization results in pronounced changes of the valence band spectra. The observed changes are explained by differences in the β -parameters of the contributing s and d initial states that result in a dichroism already without magnetic effects. The magnetic circular dichroism experiments were performed on exchange biased magnetic layers. Two types of structures were used with the MnIr (10 nm) exchange bias layer either on top or below the ferromagnetic layer. The latter were CoFe (3 nm) on-top or Co₂FeAl (30 nm) on-bottom. A pronounced magnetic dichroism of up to 50% is found at the Co and Fe $2p$ states of both materials. This demonstrates the feasibility of the method for the study of magnetism in deeply buried layers.

2A3

Depth dependence of itinerant character in $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)\text{O}_7$: evolution upon Mn doping

G Panaccione,¹ U Manju,² I Vobornik,¹ F Offi,³ L Simonelli,⁴ M A Hossain,⁵ Z Zhu,⁵ Y Yoshida,⁶ A Damascelli⁵

¹IOM-CNR, Trieste, Italy; ²ICTP, Trieste, Italy; ³Dip. Fisica Univ. Roma III, Roma, Italy; ⁴ESRF, Grenoble, France; ⁵Dep. Physics, UBC, Vancouver, Canada; ⁶AIST, Tsukuba, Japan

We present hard X-ray PES (HAXPES) data obtained at the VOLPE end-station (ESRF) from $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)\text{O}_7$, where we monitor the evolution of Ru 3d fine structure (well screened satellites) vs. Mn-doping: a clear suppression of the metallic features is observed, implying a sharp transition from itinerant to localized character. Knowing that the intensity variation of well screened peaks in HAXPES have been interpreted (in 3d-based TMO) as the result of a different screening mechanism between surface and volume [1-3], we extend this approach also to the 4d-based ruthenates and compare soft and hard X-ray data. HAXPES results reveal important changes in the degree of localized-metallic character between the surface and the bulk of the material. Our results suggest a way to control, in the same material, metallicity of the surface-interface region vs. the bulk one, by exploiting the highly sensitive response of conducting perovskites to impurities.

[1] M. Taguchi et al., Phys. Rev.Lett. **95**, 236401 [2005].

[2] K. Horiba et al., Phys. Rev.Lett. **93**, 236401 [2004].

[3] G. Panaccione et al. Phys. Rev. Lett. **97**, 116401 [2006].

2A4

Investigation of the buried silicon/zinc oxide interface by soft X-ray emission and hard X-ray photoelectron spectroscopy

M Bär,¹ M Wimmer,¹ R G Wilks,¹ D Gerlach,¹ L Weinhardt,² S Pookpanratana,³ M Blum,³ S Krause,³ Y Zhang,³ M Roczen,¹ F Ruske,¹ S Scherf,¹ R Félix,¹ C Lupulescu,¹ M Gorgoi,¹ W Yang,⁴ J D Denlinger,⁴ K Lips,¹ C Heske,³ B Rech,¹ W Eberhardt¹

¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; ²Exp. Physik VII, Universität Würzburg, Würzburg, Germany; ³Dept. of Chemistry, University of Nevada, Las Vegas, Las Vegas, United States; ⁴Advanced Light Source (ALS), Lawrence Berkeley National Laboratory, Berkeley, United States

The Si/ZnO interface plays an important role in polycrystalline silicon thin-film solar cells. For the superstrate configuration, where amorphous silicon films are deposited on the ZnO which are then subsequently solid-phase crystallized (SPC) at 600°C, potential intermixing/diffusion processes as well as chemical interactions at the interface need to be considered. For our study of the buried Si/ZnO interface, we have used soft X-ray emission spectroscopy (XES; SXF endstation, Beamline 8.0, ALS) and hard X-ray photoelectron spectroscopy (HAXPES; HIKE setup, Beamline KMC-1, BESSY). Both, our XES and HAXPES data indicates the presence of SiO_2 on the surface of the investigated Si/ZnO samples before and after SPC. Using XES, we were able to identify an SPC-induced formation of additional Si-O bonds at the Si/ZnO interface. Furthermore, the data also suggests an enhanced Zn incorporation in the Si after SPC. The complementary interface characterization by HAXPES in combination with in-situ annealing allowed to directly monitor the chemical processes taking place at the interface during SPC. In our presentation, we will paint a comprehensive picture of the chemical structure of the Si/ZnO interface and the changes induced by SPC.

2A5

X-ray absorption near edge structure and resonant X-ray diffraction simulations applied to the study of oxidesY Joly,¹ O Bunau¹¹Institut Néel, CNRS and University Joseph Fourier, Grenoble, France

We present the actual developments of the FDMNES code which allows the simulation of X-ray absorption near edge structure (XANES) spectra and Resonant X-ray Diffraction (RXD) peak intensity. The code uses both the multiple-scattering theory and the finite different method in a fully relativistic frame including thus the spin-orbit interaction. In a second step, some of the multi-electronic effects can be taken into account using the Time Dependent Density Functional Theory (TDDFT). In diffraction, the resonant and non-resonant, magnetic and non-magnetic, components are all included, allowing an easy use by the non experts. In the same idea, the automatic analysis of the unit cell (or molecule) symmetry greatly simplifies the user's work. Various examples in oxides show the potentiality of the method to get charge ordering parameters.

FOREST SCIENCES CENTRE 1005

10:40-12:30

2B1 (Invited)

Decay dynamics and nuclear motion of core-excited species probed by high resolution soft X-ray electron spectroscopyC Miron¹¹Synchrotron SOLEIL, l'Orme des Merisiers, Saint-Aubin, Gif-sur-Yvette Cedex, France

It is generally recognized nowadays that electron spectroscopy represents a powerful tool that allows investigating very accurately ultrafast decay dynamics of inner-shell excited species, especially when it is performed in ultrahigh resolution conditions. These resonant Auger Raman conditions are now routinely available at the newest soft X-ray spectroscopy facilities, such as the PLEIADES beamline at the SOLEIL synchrotron in France, which has been open to users since March 2010. For instance, such sublifetime electron spectroscopy has been applied to the case of N₂ molecule, where we were able to give evidence of a vibrational wavefunction mapping phenomenon. Indeed, the spectral shape of the resonant Auger lines fingerprints the space distribution of the square of the vibrational wave functions of the core-excited state, and thus, maps the shape of the corresponding molecular potential. Beyond the ultrahigh resolution aspects that can be exploited to study decay dynamics of small molecules, the fully variable polarization and the high flux were used to study the anisotropy of electron emission from dissociating core-excited SF₆ using circularly polarized light. Moreover, the first photoionization experiments of larger systems as large organic or biological molecules, as well as of isolated clusters and nanoparticles, were recently performed and a selection of results will be outlined.

2B2

Interatomic Coulombic decay and electron transfer mediated decay after triple ionization of Ar dimer

I Higuchi,¹ K Sakai,² T Ouchi,² H Fukuzawa,² K Ueda,² H Iwayama,³ K Nagaya,³ M Yao,³ D Zhang,⁴ D Ding,⁴ M Schoffler,⁵ T Mazza,^{2,6} Y Tamenori,¹ N Saito,⁷ S D Stoychev,⁸ A I Kuleff,⁸ L S Cederbaum⁸

¹JASRI, Sayo, Japan; ²IMRAM, Tohoku University, Sendai, Japan; ³Dept. of Phys., Kyoto University, Kyoto, Japan; ⁴Jilin University, Changchun, China; ⁵LBNL, Berkeley, United States; ⁶Univ. of Milan, Milan, Italy; ⁷NMIJ, AIST, Tsukuba, Japan; ⁸Physikalisch-Chemisches Institut, Universität Heidelberg, Heidelberg, Germany

Photoionization of Ar cluster leads to Auger decay and then may cause interatomic Coulombic decay (ICD). We have investigated these processes using electron-ion coincidence technique to get the three-dimensional momenta of ions and electrons. The experiment was carried out on the c-branch of the soft X-ray photochemistry beam line 27SU at SPring-8. We observed charge separation $\text{Ar}^{2+}\text{-Ar}^{2+}$ and $\text{Ar}^{3+}\text{-Ar}^+$ from Ar_2 after triple ionization. The $\text{Ar}^{2+}\text{-Ar}^{2+}$ separation takes place via electron transfer mediated decay, whereas the $\text{Ar}^{3+}\text{-Ar}^+$ separation takes place via interatomic Coulombic decay from $\text{Ar}^{3+}\text{-Ar}$.

2B3

Attosecond-resolved autoionization in Argon

M Chini,¹ H Wang,¹ S Chen,¹ Z Chang¹

¹J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas, United States

Bridging the gap between atomic physics and the complex systems that make up the world around us requires in-depth study of electron correlation in multi-electron systems. Fano resonances in the photoabsorption cross sections of atoms are the signature of the autoionization process, which is governed by electron-electron correlation. For decades, spectral-domain measurements with synchrotron radiation have served as a window into the rich dynamics of autoionization. However, the synchrotron pulse duration is too long (100 fs to 100 ps) to probe Fano resonances exposed to an external field in the time domain. The lifetimes of the autoionizing states of noble gases can be as short as a few femtoseconds. Here, we demonstrate that attosecond transient absorption spectroscopy can be used to probe Fano resonances in the time domain, and report the first results on time-resolved autoionization in Argon with isolated attosecond pulses. By combining isolated attosecond pulses and intense few-cycle laser pulses in a pump-probe geometry, we observed that the resonance energy, line width, and line profile of the $3s3p^6np\ ^1P_1^o$ Fano resonance series (26.7-29.2 eV) were significantly modified by the strong near infrared laser field when the delay between the XUV attosecond pulse and the laser pulse was changed by a few femtoseconds. The observed changes were strongly dependent on the laser intensity and the laser polarization. The measurement demonstrates full control of the autoionization process with attosecond precision.

2B4

Photoinduced localization and decoherence in inversion symmetric molecules

B Langer,¹ K Ueda,² U Becker^{3,4}

¹Freie Universität Berlin, Berlin, Germany; ²Tohoku University, Sendai, Japan; ³Fritz-Haber-Institut der MPG, Berlin, Germany; ⁴King-Saud-University, Riyadh, Saudi Arabia

The particle-wave dualism is most clearly exhibited by double slit experiments where the complementary quantities are localization versus coherence or in other words distinguishability in form of which-way information versus visibility in form of interference fringe contrast. In modern double-slit experiments these two behaviors may be transformed into each other. Interaction of a coherent system with the environment causes loss of coherence or decoherence thereby gaining which-way information. Imposing coherence on a localized system on the other hand erases the which-way information and gives rise to fringe patterns. One of the nicest examples of decoherence of matter waves was the gradual decoherence of C₆₀ molecules caused by thermal emission of radiation [1]. We show the decoherence of photoelectron waves by collision induced momentum kicks in the core level photoionization of N₂ [2]. This kind of decoherence behavior has been corroborated recently in strong field recollision experiments where de-Broglie dependent differences in the high harmonic generation could be revealed for the first time [3]. As a further example we present evidence for the decoherence of Auger electron waves in dissociating core-excited O₂ molecules. The decoherence of the remaining ionic system is caused by the constant velocity of the moving fragment which overtakes the tunneling motion at a certain time. In this way the still existing coherence becomes frozen and the hole state becomes localized as long as the fragments are moving. However, if this movement comes to a standstill coherence will be recovered and which-way information erased again.

[1] L. Hackermüller et al., *Nature* **427**, 711 (2004).

[2] B. Zimmermann et al., *Nature Physics* **4**, 649, (2008)

[3] H. Wörner et al., submitted to *Nature* (2010).

2B5

VUV threshold photoionization of hydrocarbon radicals

B Cunha de Miranda,^{1,2} C Alcaraz¹

¹Laboratoire de Chimie Physique, UMR 8000, CNRS et Univ. Paris-Sud 11, Orsay, France; ²Laboratório de Espectroscopia e Laser, Instituto de Física, Universidade Federal Fluminense, Niterói, Rio de Janeiro, Brazil

Hydrocarbon radicals C_xH_y[•] and their cations C_xH_y⁺ are important species in various environments such as flames, plasmas, planetary atmospheres, and interstellar medium. Because they have to be produced in situ before being studied, they are often much less characterized than stable molecules, and laboratory data are needed on these species for a better modelization of these environments. The studies of VUV threshold photoionization of small radicals presented in this work have two main goals : characterize the spectroscopy the neutral radical R and its cation R⁺, and determine the conditions to produce state-selected R⁺ cations before studying their state-specific reactivity. Two complementary source of VUV, lasers and synchrotron, are used in this work at the new Laser Center of the Paris-Sud University (CLUPS) and at the french synchrotron SOLEIL. For each VUV excitation source, appropriate threshold photoionization techniques: Pulsed Field Ionization – Zero Electron Kinetic Energy (PFI-ZEKE) and Threshold Photoelectron Spectroscopy (TPES) are used. The production of the radical beams is made by flash pyrolysis of selected organic precursors. Recent results on the VUV threshold photoionization of the methyl radical [1] and the NO molecule will be presented.

[1] Cunha de Miranda, B. K.; Alcaraz, C.; Elhanine, M.; Noller, B.; Hemberger, P.; Fischer, I.; Garcia, G.; Soldi-Lose, H.; Gans, B.; Vieira Mendes, L. A.; Boyé-Péronne, S.; Douin, S.; Zabka, J.; Botschwina, P. *J. Phys. Chem. A* **2010**, *114*, 4818.

2C1 (Invited)**Momentum dependent excitations in cuprates studied by high resolution RIXS****G Ghiringhelli¹**¹Dipartimento di Fisica - Politecnico di Milano and CNR/SPIN, Milan, Italy

The potential interest of Resonant Inelastic X-ray Scattering (RIXS) has been known since several years, but insufficient experimental energy resolution and intensity in the scattering process had been limiting the actual use of RIXS until very recently. Since then, significant technical and theoretical progress have changed the situation drastically, and high resolution RIXS measured in the soft X-ray range has become a new powerful tool in the study of 3d transition metal oxides. RIXS in the soft X-rays is ideal to probe orbital and magnetic excitations in strongly correlated systems based on 3d transition metals. I will present results obtained at the ESRF and at the SLS [1]. In particular I will show how single and multiple magnon excitations can be studied by Cu L₃ RIXS in layered cuprates (undoped and superconducting)[2,3], thus making RIXS a viable alternative to inelastic neutron scattering for the determination of spin dynamics in cuprates. The experimental results are supported by theoretical calculations combining single ion crystal field model and linear spin wave theory for 2D antiferromagnetic lattice [4].

[1] G. Ghiringhelli A. Piazzalunga, C. Dallera, *et al*, Rev. Sci. Instrum. **77**, 113108 (2006); [2] L. Braicovich, L. J. P. Ament, V. Bisogni, *et al*, Phys. Rev. Lett. **102**, 167401 (2009); [3] L. Braicovich, J. van den Brink, V. Bisogni, M. Moretti Sala, L. J. P. Ament, N. B. Brookes, G. M. De Luca, M. Salluzzo, T. Schmitt, V. N. Strocov, and G. Ghiringhelli, Phys Rev Lett. **104** 077002 (2010); [4] L.J.P. Ament, G. Ghiringhelli, M. Moretti Sala, L. Braicovich, and J. van den Brink, Phys. Rev. Lett. **103**, 117003 (2009).

2C2**First observation of two-electron one-photon transitions in single-photon impact****J Hoszowska,¹ J C Dousse,¹ J Szlachetko,^{2,3} W Cao,¹ P Jagodziński,³ Y Kayser,¹ S Nowak,¹ M Kavčič⁴**¹Physics Department, University of Fribourg, Fribourg, Switzerland; ²European Synchrotron Radiation Facility, Grenoble, France;³Institute of Physics, Jan Kochanowski University, Kielce, Poland; ⁴J. Stefan Institute, Ljubljana, Slovenia

Radiative decay of the K-shell double vacancy states proceeds mainly via the one-electron one-photon process which corresponds to the $K\alpha^h$ [$1s^{-2}1s^12p^1$] hypersatellite X-ray transition [1]. An alternative decay channel is the two-electron one-photon (TEOP) transition $K\alpha\alpha$ [$1s^{-2}2s^12p^1$] in which the two K-shell vacancies are filled simultaneously via a correlated two-electron jump [2]. This exotic decay channel provides insight into correlated multi-electron transitions. We report on the first observation of the TEOP transitions following single-photon K-shell double ionization. Measurements of the photon induced TEOP fluorescence spectra of Al and Si were carried out at the ID21 beamline of the ESRF, Grenoble, using a wavelength dispersive X-ray spectrometer [3]. The $K\alpha\alpha$ energies and the ratios of the $K\alpha\alpha$ and $K\alpha^h$ transitions were compared to available theoretical calculations. A very good agreement with the MCDF energies of Martins *et al.* [4] was found. For the branching ratios the existing theoretical predictions overestimate our experimental results.

[1] J. Hoszowska *et al.*, Phys. Rev. Lett. 102 (2009) 073006.[2] W. Wölfli *et al.*, Phys. Rev. Lett. 35 (1975) 656.[3] J. Szlachetko *et al.*, J. Synchrotron Rad. 17 (2010) [available online].[4] M. C. Martins *et al.*, J. Phys. B: At. Mol. Phys. 37 (2004) 3785.

2C3

A new method of directly determining the core-hole effect in the Ce L_3 XAS of mixed valence Ce compounds

A Kotani,^{1,2} K O Kvashnina,³ S M Btorin,³ P Glatzel⁴

¹Photon Factory, High Energy Accelerator Research Organization, Tsukuba, Ibaraki, Japan; ²RIKEN SPring-8 Center, Sayo, Hyogo, Japan; ³Department of Physics, Uppsala University, Uppsala, Sweden; ⁴European Synchrotron Radiation Facility, Grenoble, France

Using a simplified single impurity Anderson model, we calculate resonant X-ray emission (RXE) spectra with Ce $2p$ to $5d$ excitation and Ce nl to $2p$ de-excitation for mixed valence Ce compounds, where nl is $3d$ or valence states. If the core-hole effect is large to play an important role in the Ce L_3 XAS, the RXE spectral features for $nl = 3d$ and valence states are significantly different, but if it is negligibly small, they are essentially the same. Therefore, these RXE spectra are useful as a new powerful method of directly determining the core-hole effect in the Ce L_3 XAS. More detailed theoretical calculations of these RXE spectra are made for CeO₂, and compared with new experimental data, indicating the importance of the core-hole effect. Similar investigations are desirable for some metallic mixed valence Ce compounds in which the core-hole effect is controversial. We finally point out that for $nl = 5d$ we can observe the resonant inelastic X-ray scattering spectra corresponding to the charge-transfer excitations or Kondo resonance excitations.

2C4

Band-mapping and above-valence emission in Si photovoltaic materials studied using RIXS

R G Wilks,¹ J T Sullivan,² L Weinhardt,³ Y Zhang,⁴ M Blum,⁴ S Krause,⁴ B K Newman,² M Winkler,² D Recht,⁵ W Yang,⁶ M Aziz,⁵ C Heske,⁴ T Buonassisi,² M Bär¹

¹Solar Energy Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; ²Massachusetts Institute of Technology, Cambridge, United States; ³Experimentelle Physik VII, Universität Würzburg, Würzburg, Germany; ⁴Department of Chemistry, University of Nevada, Las Vegas, Las Vegas, United States; ⁵School of Engineering and Applied Sciences, Harvard University, Cambridge, United States; ⁶Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, United States

The effect of doping on the band structure of modified Si wafers is studied using Resonant Inelastic X-ray Scattering (RIXS). Si $L_{2,3}$ RIXS maps of various Si samples are presented, providing detailed electronic structure information. Subtraction of the incoherent portions of the spectra accentuates the energy loss features that trace the valence band structure; the resulting maps can be used to very accurately determine the relative energy levels needed to calculate the direct and indirect band gaps of Si-based materials. The excitation energies used to record the RIXS maps were extended past the “second threshold” – the point at which the excitation energy is sufficient to excite both a core exciton and a valence exciton – in order to separate the excitonic and band state contributions. This eliminates the overlap of the intense Rayleigh line with the much smaller inelastic spectral features. In addition to n -doped and p -doped Si standards, the band structure of silicon supersaturated with chalcogen atoms (a.k.a. “Black Si”) is studied and related to the infrared absorption that makes it an interesting material for photovoltaic and light-detecting applications. The RIXS maps exhibit sharp peaks above the valence band maximum; their intensity scales with the dopant concentration. Similar peaks have been observed in Si emission spectra but are not well understood, and the current study attempts to remove this ambiguity. We draw inferences on the possible roles of core excitons, valence excitons, and the Si valence structure on the RIXS maps.

2C5

Dispersion of two-spinon and collective orbital excitations in Sr_2CuO_3 investigated by Resonant Inelastic X-ray Scattering

T Schmitt,¹ J Schlappa,¹ K J Zhou,¹ H M Ronnow,² M Mourigal,² V N Strocov,¹ J S Caux,³ J van den Brink,⁴ L Patthey¹

¹Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland; ²Laboratory for Quantum Magnetism, EPFL, Lausanne, Switzerland; ³Amsterdam University, Amsterdam, Netherlands; ⁴IFW, Dresden, Germany

Understanding complex quantum systems that show exotic phenomena due to strong electron-electron correlations and quantum fluctuations is of pivotal importance in condensed matter physics. Resonant Inelastic X-ray Scattering (RIXS) is a powerful probe of excitations from the electronic ground state, being sensitive to spin [1], orbital and charge degrees of freedom. Here we present a high-resolution RIXS study of magnetic and electronic excitations in the low dimensional spin system Sr_2CuO_3 performed at the ADDRESS beamline of the Swiss Light Source. Sr_2CuO_3 is a corner-sharing single-chain compound possessing nearly ideal properties of the one-dimensional antiferromagnetic Heisenberg spin-1/2 model. RIXS at the Cu L_3 -edge probes the dynamical spin structure factor complementary to Inelastic Neutron Scattering. The momentum transfer dispersion of the Cu L_3 -RIXS signal along the chain direction reveals that the main spectral weight follows the lower onset of the two-spinon continuum. Line shape analysis of the RIXS response allows assessing the limits of the two-spinon dynamical spin structure factor calculated within the Bethe Ansatz. Two kinds of collective modes occur within the orbital excitation energy range, one with the same periodicity as the two-spinon spectrum and one of opposite periodicity. These results are discussed in relation to spin-charge separation and coupling between the degrees of freedom.

[1] J. Schlappa, T. Schmitt, F. Vernay *et al.*, Phys. Rev. Lett. **103**, 047401 [2009].

2C6

Coexistence of bound and virtual-bound states in shallow-core to valence spectroscopies

S S Gupta,¹ J A Bradley,² M W Haverkort,³ G T Seidler,² A Tanaka,⁴ G A Sawatzky¹

¹Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada; ²Department of Physics, University of Washington, Seattle, USA; ³Max Planck Institute for Solid State Research, Stuttgart, Germany; ⁴Department of Quantum Matter, Hiroshima University, Higashi-Hiroshima, Japan

Core-level X-ray absorption spectroscopy has played a pivotal role in the development of the present day knowledge of the electronic structure of correlated electron systems. The interpretation of such excitonic spectra relies largely on the theoretical interpretations based on local correlated models with full multiplet effects. Such models are valid, while the final state core-hole strongly binds the extra valence electron to form excitonic bound states. However, core-valence excitations within the same principle quantum number (n)-shell (3p-3d, 4d-4f, or 5d-5f), pose a problem because the core-valence multiplet spread is often much larger than the core-hole valence-electron attractive potential itself. Non-resonant inelastic X-ray scattering has at large momentum transfer the largest cross section for exactly such edges. Recent measurements show that one can obtain a wealth of information at high photon energies due to non-dipolar transitions. We develop the theory for shallow-core to valence excitations when the multiplet spread is larger than the core-hole attraction, e.g., if the core and valence orbitals have the same principal quantum number. This results in a cross-over from bound to virtual-bound excited states with increasing energy and in large differences between dipole and high-order multipole transitions, as observed in inelastic X-ray scattering. The theory is important to obtain ground state information from X-ray spectroscopies of strongly correlated transition metal, rare-earth and actinide systems.

2D1 (Invited)**Characterization of materials at high pressure with synchrotron radiation**J S Tse¹¹Department of Physics, University of Saskatchewan, Saskatoon, Saskatchewan, Canada

Pressure is a sensitive parameter for the modification of the electronic properties of a material. Using the diamond anvil cell and in combination of different synchrotron radiation techniques, the structure, dynamics and electronic properties can be measured on a very small amount of sample under extreme conditions. In this presentation, it will be shown how structural and electronic information can be extracted from these synchrotron experiments. The results will be illustrated with recent examples including the study of Mott transition in organometallic nano-magnets and novel structural transitions in elemental solids and silicon clathrates.

2D2**Electronic structure of strongly correlated materials: novel spectroscopic approaches from the VUV to the hard X-rays**L Petaccia,¹ A Barinov,¹ P Dudin,¹ S Gorovikov,¹ A Goldoni,¹ B Mansart,² F Rodolakis,^{2,3} J P Rueff,³ E Papalazarou,² M Marsi²¹Sincrotrone Trieste, Trieste, Italy; ²Laboratoire de Physique des Solides, Université Paris-Sud, France; ³Synchrotron SOLEIL, Gif-sur-Yvette, France

The study of the electronic structure of strongly correlated systems presents experimental challenges that are specific to this kind of materials. Thanks to the combined use of novel spectroscopic approaches, we were able to shine new light on a long-standing problem in this domain, namely the metal-insulator transition in the prototype Mott-Hubbard compound V_2O_3 . Low photon energy ARPES results [1] from the BaDEIPh beamline at Elettra [2] provide a deeper understanding of the nature of the surface attenuation of the quasiparticle peak in the metallic phase of V_2O_3 , which can be interpreted with a "surface dead layer" model [3]. Hard X-ray XANES on the V K-edge allowed us to compare for the first time the Mott transition induced by pressure, temperature and doping [4], finding the electronic structure of the metallic phase is non equivalent for the three cases. The reason for this unexpected behaviour can be found in the way the transition evolves on the microscopic scale, which could be studied with a novel ARPES set-up with submicron lateral resolution [5].

[1] F. Rodolakis et al., Phys. Rev. Lett. 102, 066805 (2009)

[2] L. Petaccia et al., Nucl. Instrum. Methods A 606, 780 (2009)

[3] G. Borghi, M. Fabrizio and E. Tosatti, Phys. Rev. Lett. 102, 066806 (2009)

[4] F. Rodolakis et al., Phys. Rev. Lett. 104, 047401 (2010)

[5] P. Dudin et al., J. Synchr. Rad. (2010)

2D3

Three-dimensional Fermi-surface mapping of BaFe₂As₂ using low-energy angle-resolved photoemission spectroscopy

Y Nakashima,¹ Y Utsumi,¹ H Anzai,¹ T Fujita,¹ G Hara,¹ S Nagato,¹ A Ino,¹ J Jiang,¹ H Hayashi,¹ H Iwasawa,² K Shimada,² H Sato,² M Arita,² O Morimoto,² H Namatame,² M Taniguchi,^{1,2} Y Aiura,³ A Iyo,³ H Kito,³ K Miyazawa,³ P M Shirage,³ I Hase,³ H Eisaki,³ C Lee,³ K Kihou³

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima City, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima City, Japan; ³Advanced Industrial Science and Technology, Tsukuba City, Japan

Recently the occurrence of high-T_c superconductivity in iron-based layered materials has been reported. However, the three-dimensional shape of Fermi surface remains controversial. In this work, we have studied BaFe₂As₂ by high-resolution angle-resolved photoemission spectroscopy (ARPES) using low-energy tunable photons and linearly-polarized photons, and determined the band dispersion in three-dimensional momentum space. The experiments were performed at BL-9A and BL-1 of Hiroshima Synchrotron Radiation Center. Along the Γ -X cut parallel to k_x axis, two hole-like bands, α and β , and an electron-like band, ϵ' , are observed around Γ point near the Fermi level. Scanning the photon energy $h\nu$ from 6.5 to 30 eV, we mapped out Fermi-surface cross section in k_x - k_z plane, and observed fine warping structures along k_z dispersion. The Fermi surfaces, β and ϵ' , are proximate to each other in large k_z range, indicating Fermi-surface nesting between them. The Fermi surface, α , has an egg-like shape separated at Γ and Z points with strong k_z -warping. Our results suggest that the Fermi surfaces of BaFe₂As₂ are largely reconstructed due to collinear antiferromagnetic order.

2D4

Facets, mazes, slabs, and nanowires: silver-mediated germanium growth on silicon surfaces

M Speckmann,¹ T Schmidt,¹ JI Flege,¹ I Heidmann,¹ A Kubelka,¹ A Locatelli,² TO Menten,² M Á Niño,² K Müller,¹ A Rosenauer,¹ J Falta¹

¹Institute of Solid State Physics, University of Bremen, Bremen, Germany; ²Sincrotrone Trieste, Basovizza/Trieste, Italy

The adsorption of surfactant materials on Si surfaces has a strong impact on the subsequent growth of Ge nanostructures. Due to the modulation of surface properties, like morphology and surface free energy, suppressed or enhanced 3D growth as well as less defects in the Ge structures and a reduced intermixing between Ge and the Si substrate can be observed. Hereby, we will show that Ag is an extremely versatile tool for these purposes. Depending on the substrate orientation and the Ag-induced reconstruction and morphology, either a suppressed or an enhanced 3D growth of the Ge structures can be generated. On the $\{\sqrt{3}\times\sqrt{3}\}$ -Ag reconstruction on Si(111), huge flat islands are observed with in-situ LEEM. For a growth temperature of about 500°C, the LEEM data indicate that these islands coalesce and form a continuous film at a Ge coverage of about 15 nm. XPEEM experiments give evidence for the suppression of intermixing as only a very low Si content is found in the islands. The formation of a periodic misfit dislocation network and a twin formation are observed, using GIXRD and TEM. A completely different behaviour is found for the Si(113) surface. In this case, Ag induces the formation of a regular pattern of nanofacets along the [1-10] direction. Subsequently grown Ge forms small anisotropic nanoislands with a wire-like geometry at an aspect ratio of about 4:1. These nanowires are aligned along the Ag-induced faces.

2D5

Formation of ferromagnetic metal top contacts on an organic semiconductor in soft landing conditions: evidence for a sharp, mainly nonreactive interfaceO V Molodtsova,¹ M Knupfer,² V V Kveder,³ C Laubschat,¹ V Y Aristov^{2,3}¹ISSP TU Dresden, Dresden, Germany; ²IFW Dresden, Dresden, Germany; ³ISSP RAS, Chernogolovka, Russian Federation

Recently it was shown, that Fe or Co deposited on CuPc film at RT form abrupt interface. However strong chemical interaction of Co(Fe) with the N and C of CuPc takes place. Moreover, the central Cu atoms of CuPc at the interface are reduced from Cu(II) to Cu(I), while Fe or Co atoms are oxidized and/or the ferromagnetic metals replaces this central Cu atom. In this contribution we present a detailed analysis of interfaces that are produced by deposition of the ferromagnetic elements Fe and Co onto the CuPc in UHV and using soft landing conditions. Liquid N₂ cooling provides formation of thin liquid film of xenon (condensation temperature ~166K) on CuPc substrate (creation of the condensed noble gas - Xe buffer layers of about 10 ML) before Fe or Co deposition. XPS and UPS experimental results demonstrate that at such conditions (deposition Fe or Co atoms onto CuPc film throw liquid Xe film) the unwanted chemical reactions and interdiffusion processes in the interfacial region are essentially reduced or even completely suppressed. Thus we show, that such method allows to fabricate almost ideal ferromagnetic metallic contacts, which might allow to reach the high efficiency of spin injection into unoccupied molecular orbitals of an organic semiconductor. This work was supported by the DFG under grants no. KN393/9 and KN393/14, by the RFBR under grant no. 08-02-01170 and 10-02-00269.

2D6

Molecular orientation and charge transfer dynamics studies of PTCDA on Au(111)L Cao,¹ F Xu,¹ W Zhang,¹ T Chen,¹ K Ibrahim,² H Qian,² J Wang²¹National Synchrotron Radiation Laboratory, School of Nuclear Science and Technology, University of Science and Technology of China, Hefei, Anhui, China; ²Beijing Synchrotron Radiation Laboratory, Institute of High Energy Physics, the Chinese Academy of Sciences, Beijing, China

The molecular orientation and the charge transfer dynamics of perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) molecules adsorbed on Au(111) surface have been investigated in the monolayer and multilayer regime by means of near edge X-ray absorption fine structure spectroscopy (NEXAFS) and resonant photoemission spectroscopy (RPES). All the resonances peaks from C *K-edge* NEXAFS spectra show polarization dependence, which indicate a well ordered structure for PTCDA molecules on Au(111) surface. From a quantitative analysis, the average tilt angle for the PTCDA molecular planes on the substrate Au(111) surface is $30^\circ \pm 10^\circ$ and $28^\circ \pm 10^\circ$ inclined relative to the substrate plane in the monolayer and multilayer, respectively. The charge transfer timescale, which is estimated by core-hole clock spectroscopy method based on NEXAFS and PRES technology, is on the same order of the core-hole lifetime (6fs) for C1s.

Poster Session 2P

2P - Monday, July 12, 16:10-18:00

(Setup by 10:40 on Monday, July 12, take down by 18:00 on Tuesday, July 13)

The Poster Sessions take place in the East and West Atria of the Life Sciences Institute. The conference will not be responsible for posters that are left up after the above take down times.

2P Session Topic Breakdown

SURFACES & INTERFACES

RESONANT INELASTIC SCATTERING

X-RAY EMISSION SPECTROSCOPY

HIGH ENERGY X-RAY PHOTOELECTRON SPECTROSCOPY

INSTRUMENTATION

SURFACES & INTERFACES

- 2P001 **Ning Wu**
Electron phonon coupling at the Mo(112) surface
- 2P002 **Keun Su Kim**
Nearly massless electrons in the silicon interface with a monolayer metal film
- 2P003 **Evelina Domashevskaya**
Pre-edge interference of synchrotron radiation in "silicon-on-insulator" structures
- 2P004 **Evelina Domashevskaya**
Inversion of intensity in the range of absorption edge for XANES Si L_{2,3} spectra in the structures with silicon nanocrystals
- 2P005 **Zulima Martín**
STXM spectromicroscopy of interfacial interactions in polypropylene-clay nanocomposites
- 2P006 **Kazutoshi Takahashi**
Excited electronic state on Si(001) surface at initial stage of oxidation studied by two-photon photoemission spectroscopy
- 2P007 **Maria Luiza Rocco**
Positive and negative ionic desorption from condensed formic acid photoexcited around the O 1s-edge: relevance to cometary and planetary surfaces
- 2P008 **Satoshi Kera**
Photoelectron spectra of thin film and single crystalline phase of rubrene
- 2P009 **Duorong Yuan**
Electronic structure studies of ZnAl₂O₄ nanoparticles by X-ray photoelectron spectroscopy
- 2P010 **Han-Koo Lee**
Bonding characteristics of a selenophane monolayer on Si(100)-2x1
- 2P011 **Taichi Okuda**
Direct evidence of spin-split one-dimensional metallic surface state on Au atomic chain structure on vicinal Si(111) surface
- 2P012 **Dah-An Luh**
Photon-induced rapid deterioration of metallic surfaces studied with angle-resolved photoelectron spectroscopy
- 2P013 **Koji Miyamoto**
Rashba-type spin polarization and spin-orbit-induced hybridization in surface states on W(110)
- 2P014 **Kentaro Fujii**
X-ray absorption near edge structure of DNA thin film irradiated with soft X-rays
- 2P015 **Hideki Nakajima**
Angle-resolved photoemission spectroscopy in thin Ni film on Cu(001)
- 2P016 **Intikhab Ulfat**
Synchrotron based spectroscopic investigations of continuous layers of (GaMn)As: An overview
- 2P017 **Masahiro Sawada**
Magnetic anisotropy of monoatomic Co layers on Pd(001) studied by X-ray magnetic circular dichroism
- 2P018 **Jau-Wern Chiou**
Electronic structure and characterizations of Al-doped ZnO films studied by X-ray absorption and emission spectroscopies
- 2P019 **Iwao Matsuda**
Spin-dependent interactions in quantum metal films with a Rashba-type surface

2P - MONDAY, JULY 12, 16:10-18:00 *continued*

- 2P020 **James Harries**
AlN thin film formed by exposing Al(111) to 2.0 eV N₂ molecules and studied in real time and in situ using synchrotron XPS
- 2P021 **Kazuyuki Sakamoto**
Rashba spins on heavy elements adsorbed Si surfaces
- 2P022 **Andrzej Bartnik**
EUV-induced physico-chemical changes in near-surface layers of polymers
- 2P023 **Koichiro Yaji**
Rashba spin splitting of a monolayer Pb-covered Ge(111) surface
- 2P024 **Yongfeng Hu**
Chemical characterization of SiO₂/SiC interface after nitridation treatment
- 2P025 **Yoon Hak Kim**
Hole injection enhancement for inverted organic light-emitting devices using tungsten oxide interlayer
- 2P026 **Fumihiko Matsui**
Negative contrast photoelectron diffraction replica in secondary electron angular distribution
- 2P027 **Naoyuki Maejima**
Atomic structure analysis of silicon oxynitride thin film on 6H-SiC(0001) by two-dimensional photoelectron diffraction
- 2P028 **Soon Mi Park**
Modification of cathode layer and its influence on interfacial energy level and efficiency in polymer solar cells
- 2P029 **Fabrice Bournel**
2-butyne on Si(001)-2x1 at room temperature : a XPS and NEXAFS study
- 2P030 **Ku-Ding Tsuei**
Unusually large charge transfer in C₆₀/Cu(111)
- 2P031 **Matthias Müller**
Characterization of organic surface contamination during semiconductor manufacturing processing by NEXAFS spectroscopy

- 2P032 **Yaw-Wen Yang**
Origin of high-mobility in solvent-vapor annealed anthradithiophene derivative
- 2P033 **Stéphane Carniato**
Adsorption of pyridine on Si(001)-2x1 surface revisited by theoretical simulation of XPS, polarization-dependent NEXAFS and HREELS spectra
- 2P034 **Kenichi Ozawa**
H-induced metallization of single crystal ZnO: dependence on the atomic composition of the substrate surface
- 2P036 **Alexander Gray**
Depth resolved electronic structure of an LSMO/STO superlattice via standing-wave excited angle-resolved photoemission
- 2P037 **Sergey Gorovikov**
Surface states on heavy rare earth metals
- 2P038 **Eva Benckiser**
Orbital and charge configuration in LaNiO₃-LaAlO₃ superlattices studied by X-ray resonant reflectivity

RESONANT INELASTIC SCATTERING

- 2P039 **Yoichi Isohama**
Microscopic origin of paraelectric phase transition in BaTiO₃ probed by resonant X-ray emission spectroscopy
- 2P040 **Dimosthenis Sokaras**
Resonant Raman scattering of polarized and unpolarized X-ray radiation from Mg, Al and Si
- 2P041 **Marco Moretti Sala**
dd and magnetic excitations in layered cuprates seen by high resolution Cu L₃-edge RIXS
- 2P042 **Thorsten Schmitt**
The duality of charge carriers in LaAlO₃/SrTiO₃ superlattices revealed by Resonant Inelastic X-ray Scattering
- 2P043 **Hitoshi Sato**
Polarization-dependent Ti K X-ray absorption and emission studies of Ti₂O₃ single crystal

- 2P044 **Maurits Haverkort**
Theory of resonant X-ray scattering by magnetic excitations
- 2P045 **Yasuji Muramatsu**
X-ray absorption edge of graphite evaluated from the resonance inelastic X-ray scattering and X-ray Raman scattering
- 2P046 **Matjaz Kavčič**
Characterization of 1s core-excited states of Cl containing molecules by frequency detuned resonant inelastic X-ray scattering
- 2P047 **Stéphane Carniato**
Elastic and resonant X-ray Raman scattering in the K-shell energy region of HCl
- 2P048 **Yasuhisa Tezuka**
Detailed measurement of Ti 2p resonant X-ray Raman scattering of TiO₂ and its polarization dependence measurements.
- 2P049 **Yasuhisa Tezuka**
Change of electronic structure at the ferroelectric phase transition of BaTiO₃ measured by X-ray Raman scattering
- 2P050 **Ivar Kuusik**
The sub-bandgap energy loss satellites in Be 1s RIXS spectra in beryllium compounds
- 2P051 **Ivar Kuusik**
A Ti 2p RIXS study of Ni, Co and I doped titania films
- 2P052 **Wolfgang Caliebe**
Resonant X-ray emission spectroscopy of 3d metals and oxides
- 2P053 **Wolfgang Caliebe**
Non-Resonant Inelastic X-ray scattering of cubic BN and Albite
- 2P054 **Martin Tolkiehn**
Borrmann spectroscopy - a novel tool for the analysis of quadrupole transitions
- 2P055 **Declan Cockburn**
Symmetry selective resonant X-ray emission spectroscopy study of tungsten dioxide (WO₂) at the O K-edge

X-RAY EMISSION SPECTROSCOPY

- 2P056 **Surendra Poonia**
HFS Calculation and Computed L₂ satellite spectra of ⁷⁵Re, ⁷⁷Ir and ⁷⁹Au
- 2P057 **Kiranjit Singh Kahlon**
Measurements of L₃-subshell absorption jump ratios and jump factors of Pb, Th and U
- 2P058 **Naohiro Yamaguchi**
Transmission grating spectrograph with pinhole aperture for soft X-ray spectroscopy of a laser plasma X-ray source
- 2P059 **Pascal Quinet**
Recent advances in the determination of atomic parameters for modeling K lines in cosmically abundant elements
- 2P060 **Yuka Horikawa**
Identification of electronic state of acetic acid in solution studied by X-ray emission spectroscopy
- 2P061 **Dimosthenis Sokaras**
L-shell soft X-ray emission as incident X-ray photons are tuned across 1s ionization threshold
- 2P062 **Sei Fukushima**
The change of Al L_{2,3} at the welding interface between Al and Cu
- 2P063 **Jean-Claude Dousse**
Photoinduced K_α hypersatellite X-ray emission for 12 ≤ Z ≤ 23 elements
- 2P064 **Arvo Kikas**
Comparative study of soft X-ray photoabsorption, X-ray emission and UV-VUV luminescence in BeO
- 2P065 **Nikolay Borovoy**
The features of the K-LM radiative Auger spectra of Cr, Fe, Co and Ni atoms
- 2P066 **Nikolay Borovoy**
X-ray emission M_α and M_β spectra of Au, Pb and Bi atoms under electron impact near-threshold
- 2P067 **Hidemi Arai**
Sensitivity of X-ray emission spectroscopy to hydrogen bonding: water in acetonitrile solvent

MONDAY POSTER PRESENTATIONS

2P - MONDAY, JULY 12, 16:10-18:00 *continued*

- 2P068 **Roman Ovcharenko**
Charge transfer transitions in X-ray band emission of Mg compounds
- 2P069 **Nobuo Nakajima**
Electric-field induced insulator-metal transition in a Mott insulator Ca_2RuO_4 probed by resonant X-ray emission spectroscopy
- 2P070 **Matthias Müller**
A quantitative study of the Ni-L fluorescence processes by means of high-resolution soft X-ray emission spectrometry
- 2P071 **Chung-Li Dong**
Electronic properties of $\text{FeSe}_{1-x}\text{Te}_x$ single crystals
- 2P072 **Cormac McGuinness**
The valence band electronic structure of RuO_2 - A study of chemical bonding through polarisation dependent resonant soft X-ray emission
- 2P073 **Vladimir Strocov**
Concept of spectrometer for soft-X-ray RIXS with parallel detection in incoming and outgoing photon energies

HIGH ENERGY X-RAY PHOTOELECTRON SPECTROSCOPY

- 2P076 **Irina Shabanova**
Influence of the X-ray energy on the shape of the d-metal valence bands
- 2P077 **Sven Döring**
Exploring the Fe-MgO interface using photoemission with X-ray standing-wave excitation
- 2P078 **Tiexin Chen**
Electronic structure and magnetic property of Fe-doped ZnO film grown by laser-MBE
- 2P079 **Qunfeng Xiao**
High energy photoemission spectroscopy facility at SXRMB beamline of CLS
- 2P080 **Juan Rubio-Zuazo**
Breakdown of the dipole approximation and determination of individual sub-shell cross-section for hard X-rays
- 2P081 **Ralph Claessen**
Interface-sensitive X-ray spectroscopy of oxide heterostructures: HAXPES and RIXS applied to $\text{LaAsO}_3/\text{SrTiO}_3$
- 2P082 **Mao Ye**
Hard-X-ray photoelectron spectroscopy study on role of electronic structure in the martensitic phase transition of $\text{Ni}_2\text{Mn}_{1+x}\text{Sn}_{1-x}$
- 2P083 **Hidneori Fujiwara**
Evidence for the constancy of U in the Mott transition of V_2O_3 revealed by hard X-ray Photoemission
- 2P084 **Shin Imada**
Bulk sensitive photoemission and core-level magnetic dichroism of iron
- 2P085 **Kazuma Mima**
Anisotropic occupation of orbitals in CeRh_3B_2 studied by polarization-dependent photoemission
- 2P086 **Elena Filatova**
Hard X-ray photoelectron spectroscopy as a nondestructive in-depth method for the buried interfaces study
- 2P087 **Yoshiyuki Yamashita**
Bias-voltage application in hard X-ray photoelectron spectroscopy for characterization of advanced materials
- 2P089 **Yuki Utsumi**
X-dependent electronic structure of YbXCu_4 (X=Cd, In, Sn) investigated by hard X-ray photoemission spectroscopy
- 2P090 **Keisuke Kobayashi**
Hard X-ray photoelectron spectroscopy, first principle calculation, and chemical bonding in phase change memory materials $(\text{GeTe})_{1-x}(\text{Sb}_2\text{Te}_3)_x$

- 2P091 **Masaaki Kobata**
Development of laboratory hard X-ray photoelectron spectroscopy system and application to measurement of SiO₂ thickness on Si(001)
- 2P092 **Alexander Foehlisch**
Hard X-ray high kinetic energy photoelectron spectroscopy in BESSY II - recent results
- 2P093 **Andrey Pavlychev**
Vibrational structure of the C 1s⁻¹ photoelectron line of CO
- 2P094 **Igor Pis**
Photoelectron diffraction patterns from ZnO and Si single crystals at high kinetic energies
- 2P095 **Alexander Gray**
Bulk electronic structure of [Ga,Mn]As ferromagnetic semiconductors via angle-resolved hard X-ray photoemission
- 2P096 **Alexander Gray**
Hard X-ray photoemission measurement of the band gap in an epitaxial, semiconducting Cr_{0.80}Al_{0.20} thin film
- 2P097 **Alexander Gray**
Hard X-ray photoemission study of Fe_{1-x}Si_x binary Heusler alloys
- 2P098 **Alexander Gray**
Electronic properties of LaNiO₃ Mott interfaces via hard X-ray photoemission
- 2P099 **Alexander Gray**
Bulk electronic structure and recoil effects in LaB₆ via hard X-ray photoemission and hard X-ray ARPES
- 2P100 **Wolfgang Drube**
Hard X-ray photoelectron spectroscopy at PETRA III
- 2P101 **Vladimir Strocov**
Soft-X-ray ARPES endstation at the ADDRESS beamline of Swiss Light Source

INSTRUMENTATION

- 2P102 **Urs Wiesemann**
Plasma based XUV sources and solutions: Synchrotron beamline and endstations supplement for the lab
- 2P103 **Fred Bijkerk**
Progress in multilayer XUV reflecting Bragg optics

2P001

Electron phonon coupling at the Mo(112) surfaceN Wu,¹ YB Losovyj,² PA Dowben¹¹Physics and Astronomy, Lincoln, Nebraska, United States; ²Center For Advanced Microstructures and Devices, Louisiana State University, Baton Rouge, Louisiana, United States

We have investigated the electron-phonon coupling (EPC), in the vicinity of the Fermi level, for the surface states and bulk states of Mo(112). These high resolution angle resolved photoemission data were taken parallel to the surface corrugation of surface. Analysis of experimentally determined self energy provides the mass enhancement factor $\lambda=0.389$ through fitting with Debye model. The band width is discussed in terms of electron-electron interactions, electron impurity scattering and electron phonon coupling. The bulk band widths in the vicinity of the Fermi level are dominated by the oscillatory interlayer spacing in the region of the surface. This oscillatory interlayer spacing in the region of the surface results in multiple bulk bands, and is similar to the multiple core level peaks observed for some metals with significant oscillatory interlayer spacing in the region of the surface. The "fine structure" in the band structure mapping are a further indication that corrections must be included for the lattice relaxation of the Mo(112) surface. In the case of Mo(112) the surface layer relation is significant: the first layer contraction has been experimentally determined to be 14.9%, in general agreement with the calculated 17.6% contraction from total surface energy optimization [1].

[1] N. Wu, Ya. B. Losovyj, Z. Yu, R.F. Sabirianov, W. N. Mei, N. Lozova, J.A. Colón Santana, and P.A. Dowben, *J. Phys. Cond. Matter* 21 (2009) 474222

2P002

Nearly massless electrons in the silicon interface with a monolayer metal filmKS Kim,¹ SC Jung,² MH Kang,² HW Yeom¹¹Institute of Physics and Applied Physics and Center for Atomic Wires and Layers, Yonsei University, Seoul, Republic of Korea; ²Department of Physics, Pohang University of Science and Technology, Pohang, Republic of Korea

Massless electrons are attracting tremendous interest owing to their extremely high mobility useful for high-performance electronic devices [1]. The notable feature of massless electrons stems mainly from linear energy dispersion, distinguished from parabolic dispersion in ordinary semiconductors with finite-mass electrons. However, electrons with linear dispersions have been found in extremely limited materials systems, only in graphene [2] and bismuth compounds [3,4], where difficulties exist in promptly realizing practical devices. In this presentation, we show the realization of nearly massless electrons in the most widely used device material, silicon, at its interface with a monolayer metal film. Using angle-resolved photoemission, we found that the surface band of a monolayer metal film drives a hole band of Si inversion layers formed at the interface with the film to have nearly linear dispersion with an extremely small effective mass. The reduction of mass can be accounted for by repulsive interaction between neighboring bands of a metal film and a Si substrate, as modeled well by *k-p* perturbation theory [5]. Our result suggests a promising way to take advantage of "ultrafast" carriers in silicon-based thin-film devices, which can also be applied for various other semiconductors.

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2P003

Pre-edge interference of synchrotron radiation in "silicon-on-insulator" structuresEP Domashevskaya,¹ SY Turishchev,¹ VA Terekhov¹¹Solid State Physics and Nanostructures Department, Voronezh State University, Voronezh, Russian Federation

An interference of synchrotron radiation is observed in silicon nanolayer deposited on the dielectric layer of SiO₂ (~150 nm) on a single-crystalline substrate of Si (100) (structure of silicon-on-insulator "SOI") for the first time. Investigations of this effect using XANES (X-ray adsorption near edge structure) technique near L_{2,3} - absorption edge of silicon were performed at SRC synchrotron (Stoughton, USA). Angular dependence of XANES spectra with $\theta=2^\circ$ step was obtained at RGLB beamline of BESSY II synchrotron (Berlin, Germany). Abrupt changes of spectral intensity in a dependence of the photons energy were observed in the fine structure of the quantum yield of X-ray photoeffect in the energy range preceding Si L_{2,3} absorption edge of the elementary silicon ≤ 100 eV for the grazing angles $\theta < 21^\circ$. For small changes of the angle ~ 2 in the interval of $4^\circ < \theta < 21^\circ$ the phase of the oscillating structure of the spectrum is changed to the opposite one. Basing on position of the neighboring peaks of interference for ultrasoft X-ray radiation in XANES spectra an estimation of thickness for silicon nanolayer (~80 nm) was made in a three-layer structure of strained Si - SiO₂ - Si substrate. Decrease of the lattice parameter in the nanolayer of strained silicon in the direction normal to the substrate was determined by X-ray diffraction technique. USXES (Ultrasoft X-ray emission spectroscopy) technique allows to determine an increase of interatomic Si-Si distances in the distorted lattice of strained silicon for SOI structure.

This work is based upon research supported by the Federal Targeted Program "Scientific and Scientific-Educational Personnel of the Innovative Russia".

2P004

Inversion of intensity in the range of absorption edge for XANES Si L_{2,3} spectra in the structures with silicon nanocrystals

VA Terekhov,¹ SY Turishchev,¹ KN Pankov,¹ IE Zanin,¹ EP Domashevskaya,¹ DI Tetelbaum,² AN Mikhailov,² AI Belov,² DE Nikolichev,² SY Zubkov²

¹Solid State Physics and Nanostructures Department, Voronezh State University, Voronezh, Russian Federation; ²Semiconductor physics and optoelectronics department, N.Novgorod State University, N.Novgorod, Russian Federation

The investigations of nanomaterials and nanostructures by near-edge X-ray absorption fine structure technique in the last years are of a great interest since they provide information on the local atomic structure. A considerable role in these investigations belongs to a close value of the wave-lengths in the ultrasoft range and characteristic size of structural inhomogeneities in nanomaterials. As a result this can lead to appearing of interference and diffraction effects on the structural inhomogeneities under investigations with the use of synchrotron radiation [SR] in the range of nanometer wave-lengths. Formation of nanocrystals of the elementary silicon in the films of silicon sub-oxide SiO_x on Si(111) substrate after thermal anneals at 900-1100 C was investigated using XANES, XPS and XRD techniques. The most interesting and unusual results were obtained basing on Si L_{2,3} XANES data. Well-expressed inverse fine structure of the total quantum yield was observed in XANES spectra of the films after their annealing in the range of photon energies $h\nu \approx 100-104$ eV, i.e. in the range of elementary silicon Si L_{2,3} absorption edge. Anomalous behaviour of XANES can be observed over rather large interval of the grazing angles $\sim 30-90^\circ$ and this can be due to the interference of synchrotron radiation at nanocrystals with a thickness of 3-6 nm. XPS data show that SiO_x:ncSi/Si(111) films have rather thick layer of pure oxide of about 60 nm on the surface. Elementary silicon could be also found along with the oxide at the depth of about 60 nm with the binding energy of Si 2p - level 99.3 eV. This work is based upon research supported by the Federal Targeted Program "Scientific and Scientific-Educational Personnel of the Innovative Russia".

2P005

STXM spectromicroscopy of interfacial interactions in polypropylene-clay nanocomposites

Z Martín,¹ I Jiménez,² MA Gómez,³ AP Hitchcock¹

¹Department of Chemistry and BIMR, McMaster University, Hamilton, Ontario, Canada; ²Instituto de Ciencia de Materiales de Madrid, (ICMM), CSIC, Madrid, Spain; ³Instituto de Ciencia y Tecnología de Polímeros (ICTP), CSIC, Madrid, Spain

When adding layered silicate nanoclays to polymers, the high surface area of these nanoparticles increases the interfacial interactions between matrix and clay. Thus, improvements in material properties (gas permeability, thermomechanical behaviour) will depend strongly on these interactions. In this system, the polar character of the silicates and the non-polar nature of the polypropylene matrix make necessary the incorporation of compatibilizing agents. We have used soft X-ray scanning transmission microscopy (STXM) to investigate nanocomposites of polypropylene matrix (PP), poly(styrene-*b*-ethylene-butylene-*b*-styrene) (SEBS) and montmorillonite (MMT), made by melt processing, using as additives polypropylene-graft maleic anhydride (PP-*g*-MA) and polymeric components (PP and SEBS) surface modified by N₂-plasma treatment. Quantitative chemical maps from STXM based on C 1s X-ray absorption spectra provide direct visual and compositional chemical information of the polymer-silicate interfaces. Combining the STXM results with those from XRD, SEM and TEM microscopies, provides insight into the interactions between the different components.

2P006

Excited electronic state on Si(001) surface at initial stage of oxidation studied by two-photon photoemission spectroscopy

K Takahashi,¹ Y Kurahashi,¹ T Koga,¹ J Azuma,¹ M Kamada¹

¹Synchrotron Light Application Center, Saga University, Saga, Japan

Electronic structure of ultrathin silicon oxide film and its initial growth stage have been extensively studied since they play a key role in the present and near future metal-oxide semiconductor devices. Up to now, their occupied electronic structures have been studied by means of some electron spectroscopic techniques such as the photoemission spectroscopy. On the other hand, knowledge about the unoccupied states above the Fermi level and temporal electron dynamics is scarce to date. In this work, the excited electronic state on Si(001) surface at the initial oxidation stage has been studied by time-resolved two-photon photoemission spectroscopy. The experiments have been performed at Saga University beamline in Saga Light Source. The samples have been prepared *in-situ* by thermal oxidation at the substrate temperature of 600 °C and the exposure to oxygen of up to 150L. The prepared samples have been characterized by Si 2p and valence band photoemission measurements with synchrotron radiation. The time-resolved two-photon photoemission (2PPE) measurements have been performed with using the frequency-doubled and tripled light of Ti:Sapphire regenerative amplifier as the excitation source. Temporal 2PPE intensity at the intermediate energy corresponding to the conduction band minimum [CBM] shows maximum at about 1 ps after the excitation by pump pulse. This is due to the accumulation of photoexcited electrons to CBM by intraband scattering. The intensity around 0.6 eV below CBM shows maximum intensity at 2 ps. It is considered that this 2PPE intensity originates from unoccupied surface states located in the bulk band gap. It has been found that transient 2PPE intensity and its low energy cutoff show the explicit dependence on the amount of the oxidation.

2P007

Positive and negative ionic desorption from condensed formic acid photoexcited around the O 1s-edge: relevance to cometary and planetary surfaces

DPP Andrade,¹ HM Boechat-Roberty,¹ EF da Silveira,² MLM Rocco¹¹Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil; ²Pontifical Catholic University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil

Photon stimulated ion desorption (PSID) studies have been performed in condensed formic acid using oxygen 1s-edge synchrotron radiation from the Brazilian Synchrotron Light Source (LNLS) operating in a single-bunch mode and employing time-of-flight mass spectrometry (TOF-MS) for ion analysis. While the positive PSID spectrum is rich, presenting many features, the negative spectrum shows only H⁺ and O⁻ species. Ion formation was discussed in terms of the Auger Stimulated Ion Desorption (ASID) and X-ray induced electron stimulated desorption (XESD) mechanisms. The photon energy dependent studies revealed that C⁺, CH⁺, O⁺, O⁻ and H⁺ desorptions occur mainly via ASID mechanism, while for other fragments the contribution due to XESD process has to be invoked. The hydroxyl anion has not been observed while the hydroxyl cation showed low intensity or was absent. Some anion formation routes from dissociative reactions are suggested taking into account the positive ion yields. The authors acknowledge LNLS, CNPq, FAPERJ and CAPES for financial support.

2P008

Photoelectron spectra of thin film and single crystalline phase of rubrene

S Kera,¹ S Machida,¹ Y Nakayama,¹ A Funakoshi,¹ N Ogawa,¹ S Hosoumi,¹ Q Xin,¹ S Duhm,¹ H Ishii,¹ N Ueno¹¹Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

The mechanism of the carrier transport in organic semiconductor has remained a puzzling at room temperature region, especially. Rubrene (C₄₂H₂₈) single crystal has been recognized to exhibit the highest hole mobility among all organic semiconductors [1]. To comprehend the transport nature as well as to improve the device performance, information on the electronic structure is indispensable. In the present study, we successfully observed the valence electronic structures of rubrene single crystal by angle-resolved ultraviolet photoelectron spectroscopy with laser illumination to avoid sample charging. A clear energy dispersion of the highest occupied molecular orbital band was observed, where the dispersion width is 0.4 eV along the well conjugated direction. Effective mass of holes is estimated to be 0.65 m₀. The present results suggest that the carrier conduction mechanism in a rubrene single crystal should be described as band transport of a delocalized light quasiparticle [2].

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2P009

Electronic structure studies of ZnAl₂O₄ nanoparticles by X-ray photoelectron spectroscopy

D Yuan,¹ X Duan¹¹Shandong University, State Key Laboratory of Crystal Materials, Jinan, Shandong, China

X-ray photoelectron spectroscopy (XPS) was used to study the electronic structure of ZnAl₂O₄ nanoparticles for the first time. The results show that the divalent Zn²⁺ ions primarily occupy tetrahedral sites in ZnAl₂O₄ nanoparticles, but there is a little number of Zn²⁺ ions entering octahedral sites. The inversion parameter increases with calcination temperature increasing. The XPS spectrum of Al2p can be deconvoluted into two peaks, which indicates that Al³⁺ ions occupy two different coordination sites in ZnAl₂O₄ nanoparticles. The O1s spectrum is composed of two peaks: the main lattice peak at 531.31 eV, and a component at 529.12 eV, which is believed to be intrinsic to the sample surface. The result revealed the characteristic of surface structure of ZnAl₂O₄ nanoparticles. This work can provide the basis for the doping and modification of ZnAl₂O₄ nanomaterials.

2P010

Bonding characteristics of a selenophane monolayer on Si(100)-2x1

HK Lee,¹ KJ Kim,¹ HD Kim,¹ HJ Shin,^{1,2} IJ Lee,¹ B Kim,^{1,2} JW Chung²¹Pohang Accelerator Laboratory, Pohang, Kyung-Buk, Republic of Korea; ²Departments of Physics, POSTECH, Pohang, Kyung-Buk, Republic of Korea

We have investigated the adsorption of selenophene molecules on the Si(100)-2x1 surface at room temperature by using near-edge X-ray absorption fine structure (NEXAFS) and high resolution photoemission spectroscopy. The Si 2p, C 1s, Se 3d core-level spectra reveal that the selenophene molecules are chemisorbed non-dissociatively through the [2+2] cycloaddition on the Si(100)-2x1 surface, and form a uniform selenophene monolayer upon annealing at 350 K. The π* orbitals of C=C bonds is found to show a good angular dependence in the carbon K-edge NEXAFS spectra from which we obtain an average tilting angle α ~ 53 ± 3° for the aromatic ring plane of the selenophene monolayer with respect to the surface normal. Such a bond geometry is consistent with the [2+2] cycloaddition of selenophene, forming a Si₂C₂ four-membered ring.

2P011

Direct evidence of spin-split one-dimensional metallic surface state on Au atomic chain structure on vicinal Si(111) surface

T Okuda,¹ K Miyamoto,¹ Y Takeichi,² H Miyahara,³ A Harasawa,² I Matsuda,² A Kakizaki,² T Shishidou,⁴ T Oguchi⁴

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan; ³School of Science, Hiroshima University, Higashi-Hiroshima, Japan ⁴Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima, Japan

Au evaporation on Si(111) vicinal surfaces results in the one-dimensional Au chain structure having one-dimensional electronic structure[1]. Interestingly, the one-dimensional metallic surface states consist of proximal double parabolic bands. The origin of this double bands, however, is still in controversy. Here we report unprecedented evidence of a spin-split in the one-dimensional metallic surface states by means of high-resolution spin-and angle-resolved photoelectron spectroscopy (SARPES) combined with first principles calculation. A reversal of the spin polarization with respect to the time-reversal symmetry point as is characteristic from the Rashba effect has been clearly observed. Moreover, we have observed a considerably large out-of-plane spin polarization which we attribute to the highly anisotropic wave function of the gold chains suggested by our first principles calculation. These findings allows us to shed some light over the controversial nature of these surface states, finally settling this matter as originating from a Rashba effect. The demonstration of locked dominant out-of-plane spin polarization in one-dimensional metallic surface states due to restricted electron momentum will very likely stimulate revitalized research in metallic one-dimensional systems for the spintronics devices. [1] J.N. Crain et al., Phys. Rev. B 69, 125401 (2004).

2P012

Photon-induced rapid deterioration of metallic surfaces studied with angle-resolved photoelectron spectroscopy

DA Luh,^{1,2} KC Liu,¹ CM Cheng,² KD Tsuei²

¹Department of Physics, National Central University, Taoyuan, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan

We report rapid deterioration of metallic surfaces induced by photon irradiation at low temperature. The surface of interest is Cu(111), but a Cu(111) surface partially covered with Ag was chosen for testing. The surface of Ag/Cu(111) is characterized with its Shockley states with angle-resolved photoelectron spectroscopy. We observed a rapid degradation of the Shockley state of Cu(111) during photoemission at temperatures less than 220 K. A different evolution of the Shockley states during annealing and cooling was also discovered. All these observations favor a mechanism based on photon-stimulated chemisorption of hydrogen on the surface. We suggest that this mechanism of surface deterioration affects all investigations of a surface involving intense radiation, but its influence varies with several factors. [1] D.-A. Luh, K.-C. Liu, C.-M. Cheng, and K.-D. Tsuei, Phys. Rev. B 81, 035427 (2010).

2P013

Rashba-type spin polarization and spin-orbit-induced hybridization in surface states on W(110)

K Miyamoto,¹ A Kimura,² M Donath,³ J Braun,⁴ K Kuroda,² T Okuda,¹ H Namatame,¹ M Taniguchi^{1,2}

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ³Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Münster, Germany; ⁴Department Chemie und Biochemie, Lehrbereich Physikalische Chemie, Ludwig-Maximilians-Universität München, München, Germany

Spin-orbit effects such as the Rashba effect are expected to play a considerable role in spintronics technology in order to control spin orientation and spin current without a magnetic field[1]. Tungsten is well known as a prototype material for spin-orbit effects during the last decades[2]. Previous work on clean W(110) with spin-integrated angle-resolved photoelectron spectroscopy (ARPES) revealed a surface state around $\bar{\Gamma}$ -bar within a spin-orbit-induced energy gap for bulk states of a certain symmetry[3]. More surface states on the Fermi surface of W(110) have been identified[4] but no information about the spin polarization of these surface states is available so far. In the present study, we have characterized the spin polarization of several surface states of W(110) along the $\bar{\Gamma}$ -bar-N-bar line by means of spin-resolved ARPES. Our angle-resolved results show that the surface state exhibits a clear Rashba-type spin polarization when it enters a total energy gap, while the spin polarization is much weaker when the surface state appears only in a symmetry gap. This indicates that the spin-orbit-induced hybridization between bulk and surface states of otherwise symmetry-separated states causes surface states to become surface resonances and, therefore, reduces the spin polarization. Our results have clarified how spin-orbit induced hybridization affects the spin polarization of the surface states of W(110). [1] S. Datta et al., APL 56, 665 (1990). [2] J. Kirschner et al., PRL 42, 1008 (1979). [3] R. H. Gaylord et al., PRL 62, 2036 (1989). [4] E. Rotenberg et al., PRL 80, 2905 (1998).

2P014

X-ray absorption near-edge structure of DNA thin film irradiated with soft X-raysK Fujii,¹ A Yokoya¹¹Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Naka, Ibaraki, Japan

Soft X-rays produce a variety of molecular change (damage) in cellular DNA, which is thought to be the critical target of the biological effects of radiation, such as mutation induction. Recently, we have reported the yields of base lesions as well as strand breaks strongly depend on soft X-ray energy around carbon (C), nitrogen (N) and oxygen (O) K-edge regions. The K-shell ionization of oxygen most likely contributes to the induction of nucleobase lesions. DNA single strand breaks, on the other hand, are preferably produced just below N K-edge. Therefore, we have concluded that the kinds of DNA damage can be selectively induced by monochromatic soft X-ray irradiation. To investigate the mechanism of the molecular change in DNA irradiated with the soft X-rays, we have measured the spectra of the X-ray absorption near edge structure (XANES) of DNA caused by exposure to monochromatic soft X-rays. We used a calf thymus DNA and oligonucleotide thin films as samples and observed N K-shell and O K-shell XANES spectral changes. The typical monochromatic soft X-ray energies used for the irradiation (380, 435, 560, and 760 eV, $E < 0.1$ eV) were obtained from SPring-8, BL23SU. The observed spectra showed that initiation of the new products by the irradiation in the irradiated sample and the dissociation of molecular structure of the DNA by the irradiation. By comparison of these XANES spectral changes with the yields of base lesions and strand breaks as final products, we will discuss the molecular structure of DNA damage site and the site selectivity of damage induction in DNA by soft X-rays.

2P015

Angle-resolved photoemission spectroscopy in thin Ni film on Cu(001)H Nakajima,^{1,2} R Supruangnet,³ R Chai-ngam,¹ P Songsiriritthigul,^{1,2,3} A Kakizaki⁴¹Synchrotron Light Research Institute, Nakhon Ratchasima, Thailand; ²ThEP Center, Commission on Higher Education, Bangkok, Thailand; ³School of Physics, Suranaree University of Technology, Nakhon Ratchasima, Thailand; ⁴Institute for Solid State Physics, The University of Tokyo, Chiba, Japan

We discuss the origin of the perpendicular magnetic anisotropy (PMA) based on the spin-orbit coupling where $d_{x^2-y^2}$ and d_{z^2} orbitals contribute to the perpendicular and in-plane magnetic anisotropies. Recently, it was found that in thin Ni films on a Cu(001) substrates, the d electron spins stabilize to the surface perpendicular direction due to the increase of $d_{x^2-y^2}$ orbital occupancy, which is corresponding to the first spin reorientation transition. In this report, we provide a clue to discuss how PMA switches back to the in-plane magnetic anisotropy in thick Ni films, which is called the second spin reorientation transition. The electronic structures were studied by both angle-resolved photoemission spectroscopy and a first-principle energy-band calculation in the thickness range up to Ni 30 ML.

2P016

Synchrotron based spectroscopic investigations of continuous layers of (GaMn)As: an overviewI Ulfat,^{1,2,3} J Adell,² J Sadowski,² L Ilver,¹ J Kanski¹¹Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden; ²MAX-lab, Lund, Sweden; ³Department of Physics, University of Karachi, Karachi s, Karachi, Pakistan

We present a summary of our research regarding the MBE growth and synchrotron-based characterization of continuous layers of (GaMn)As carried out at the Swedish National Facility of Synchrotron Radiation-MAX-lab. The ultimate aim of these studies is to achieve basic understanding and optimization of the properties of (GaMn)As. (GaMn)As is a model diluted ferromagnet system in which the atomic spins of Mn ions are ferromagnetically arranged due to the exchange interaction with valence band. Concerning the homogenous (GaMn)As layers we have followed different approaches that might result in reduction of the density of Mn interstitial and increase in the content of Mn. We highlight our recent results concerning annealing induced modifications in (GaMn)As layers. We also present an account of our successful RIXS measurements of the system. In the end, we emphasize a couple of vital modifications pertaining the instrumentation side. These changes will certainly improve the opportunity to accomplish novel results in an unswerving manner with greater efficiency. Firstly a new beamline on MAX III is now in operation allowing us to study the electronic structure with a much higher energy resolution than was possible until now, and to obtain spin-resolved spectra. The other improvement is a new MBE facility that offers the growth of graded structures giving the choice to examine the thickness and doping dependence more effectively.

2P017

Magnetic anisotropy of monoatomic Co layers on Pd(001) studied by X-ray magnetic circular dichroism

M Sawada,¹ T Tagashira,² K Furumoto,² T Ueno,² A Kimura,² H Namatame,¹ M Taniguchi^{1,2}

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan

L10-type ordered alloys composed of a ferromagnetic transition metal and a noble metal have attracted much attention for the last decade because of their own magnetic property. The films of the ordered alloys show perpendicular magnetic anisotropy (PMA), which is crucially important in development of high-density magnetic recording media. In order to understand PMA origin from a viewpoint of electronic structure, we have focused on ultrathin film structures with a Co monolayer on Pd(001), which are one of ideal ultrathin film systems for the research on PMA. Previous studies revealed that the as-grown 1 ML Co/Pd(001) film shows in-plane magnetic anisotropy and perpendicular magnetization appears in the monoatomic sandwiched structure of Pd/Co/Pd(001). We carried out in-situ experiment of the monoatomic films fabrication and the electronic structure survey at the soft X-ray beamline HiSOR-BL14. We fabricated both the as-grown and sandwiched structures of the Co monolayer films on the Pd substrate, and closely investigated the spin and orbital magnetic moment at the Co atomic site by means of X-ray magnetic circular dichroism (XMCD) spectroscopy as well as the macroscopic property of the magnetic anisotropy. From our detailed analysis of the XMCD spectra, we conclude that the anisotropy of orbital magnetic moment plays crucial role to decide magnetic anisotropy in this system.

2P018

Electronic structure and characterizations of Al-doped ZnO films studied by X-ray absorption and emission spectroscopies

JW Chiou,¹ H Chou,² WF Pong,³ J Guo⁴

¹Department of Applied Physics, National University of Kaohsiung, Kaohsiung, Taiwan; ²Department of Physics, National Sun Yat-sen University, Kaohsiung, Taiwan; ³Department of Physics, Tamkang University, Taipei, Taiwan; ⁴Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, United States

Al-doped ZnO (AZO) transparent conductive thin films have been prepared on glass substrates by direct current magnetron sputtering. High purity Ne (5N) was used as the sputtering gas. X-ray absorption near-edge structure (XANES) and X-ray emission spectroscopy (XES) measurements were used to investigate the effect of transparent and conductive AZO thin films. The XANES spectra of AZO thin films reveal the decrease of the number of both O 2p and Zn 4s/3d unoccupied states with the increase of the pressure of Ne. The number of Al 3p unoccupied states increases when the pressure of Ne increase, indicating that Al doping increased the negative effective charge of oxygen ions through Al 3p-O 2p hybridization. XANES and XES spectra of O 2p states indicate that Al doping not only raises the conduction-band-minimum but valence-band-maximum and increases the band gap.

2P019

Spin-dependent interactions in quantum metal films with a Rashba-type surface

H Ke,¹ Y Takeichi,¹ T Okuda,¹ M Ogawa,¹ A Harasawa,¹ P Moras,² D Topwal,³ C Carbone,² A Kakizaki,¹ I Matsuda¹

¹the Institute for Solid State Physics, the University of Tokyo, Chiba, Japan; ²Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy; ³International Centre for Theoretical Physics, Trieste, Italy

In the present research, we combined the two quantum effects of quantum size effect and Rashba effect by preparing a quantum film, the ultrathin Ag(111) film, covered with a Rashba-type surface, the $\sqrt{3} \times \sqrt{3}$ -Bi/Ag ordered alloy. Then, we investigated the spin-polarized electronic structure by means of spin- and angle-resolved photoemission spectroscopy. Spin-degenerate QWS and spin-split SS bands hybridize selectively, as dictated by their relative spin orientation and symmetry properties. The bands form energy gaps only when spins of the QWS and SS bands are parallel. Appearances of level crossing and anti-crossing were found between the QWS and SS bands that can be understood in terms of symmetry of the wave functions. The present spin-resolved photoemission analysis directly proves that spin control in non-magnetic nanostructures can be achieved by properly designing spin-orientation and symmetry of the electronic states in the interface atomic layer.

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2P020

AlN thin film formed by exposing Al(111) to 2.0 eV N₂ molecules and studied in real time and in situ using synchrotron XPS

JR Harries,¹ Y Teraoka,¹ A Yoshigoe¹

¹Japan Atomic Energy Agency, SPring-8, Japan

While clean surfaces of aluminium react readily with oxygen they are inert to nitridation under normal conditions. AlN has many applications, and its formation usually requires the use of techniques such as metal-organic vapour-phase epitaxy. We have found however [1] that a film of AlN can be formed on simple exposure to a beam of energetic (>1.8 eV) nitrogen molecules. The nitridation is carried out *in situ* at BL23SU, SPring-8, monitoring the surface coverage in real time during exposure using photo-electron spectroscopy. The overall energy resolution is sufficient to resolve 4 components in the N 1s photo-electron peak, which can be assigned to intermediate nitride states. The evolution of these components is followed during the reaction. A linear dependence on dose is observed, indicating that unlike in oxidation, a protective film is not formed, and suggesting significant penetration. By recording spectra at several take-off angles following exposure a chemical-state specific depth-profile is generated, confirming these observations.

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2P021

Rashba spins on heavy elements adsorbed Si surfaces

K Sakamoto,¹ A Kimura,² T Oda,³ K Miyamoto,² T Kuzumaki,¹ T Takahashi,⁴ J Fujii,⁵ T Oguchi,⁶ RIG Uhrberg⁷

¹Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ³Graduate School of Natural Science and Technology, Kanazawa University, Kanazawa, Japan; ⁴Department of Physics, Tohoku University, Sendai, Japan; ⁵TASC National Laboratory, INFN-CNR, Trieste, Italy; ⁶Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima, Japan; ⁷Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden

The Rashba-Bychkov (RB) effect is one of the novel exotic solid-state properties observed when decreasing the size of a crystal to nanometer scale. The spin-split band structures originating from the RB effect has been observed on clean noble metal surfaces and heavy group V elements, and has recently been reported to be enhanced in systems in which heavy element atoms are adsorbed on light element substrates. The spin-split bands reported in these former studies show similar behaviors as those of the simple RB effect. In this paper, we will present our studies on heavy elements adsorbed Si surfaces, and show that the symmetry of the surface, which was not considered earnestly, would lead to the appearance of peculiar RB spins that was not reported in any 2D or 3D system so far. In the case of a threefold symmetric surface, the spin polarization vector of the RB spin was observed to change abruptly to the surface normal direction at a symmetry point of the surface Brillouin zone with C₃ symmetry, and a peculiar vortical RB splitting was observed even at a point without time-reversal invariance when its symmetry is C_{3v}. We will also present our results on heavy elements adsorbed twofold and fourfold symmetric Si surfaces. All the novel quantum phenomena are corroborated by the combination of high-resolution angle-resolved photoemission and spin-resolved photoemission measurements, and a state-of-the-art theoretical calculation.

2P022

EUV-induced physico-chemical changes in near-surface layers of polymers

A Bartnik,¹ H Fiedorowicz,¹ R Jarocki,¹ J Kostecki,¹ M Szczurek,¹ O Chernyayeva,² JW Sobczak²

¹Institute of Optoelectronics, Military University of Technology, Warsaw, Poland; ²Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland

In this work a laser-plasma EUV source based on a gas puff target was used for micro- and nanostructuring of polymer foils. The plasma radiation was focused using a gold-plated grazing incidence ellipsoidal collector. The collector allowed for effective focusing of radiation of Kr plasma within the wavelength range 9 – 70 nm. The polymer foils were irradiated in the focal plane or at some distance downstream the focal plane of the EUV collector. The surface morphology of the irradiated polymer samples was investigated using a scanning electron microscope (SEM) and atomic force microscope (AFM). The chemical changes were investigated by X-ray photoelectron spectroscopy (XPS). Different kinds of micro- and nanostructures created in near-surface layers of different kinds of polymers were obtained. Form of the structures depend on a particular polymer and irradiation parameters. In most cases exposure with the fluence close to the maximum resulted in ablation or formation of different kinds of microstructures. Exposure with relatively low fluence and large number of EUV pulses resulted in different kinds of nanostructures. In a case of PET irradiated and soaked in acetone, different kinds of nanostructures were created even after a single pulse. Concerning changes in a chemical structure XPS spectra coming from different chemical states of carbon C1s and oxygen O1s were measured. Analysis of the spectra gave information on C/O relative concentrations and changes in molecular bonds in the near surface layer. Significant differences were revealed in XPS spectra corresponding to the valence bands between irradiated and not-irradiated polymer.

2P023

Rashba spin splitting of a monolayer Pb-covered Ge(111) surface

K Yaji,^{1,2} Y Ohtsubo,^{1,2} S Hatta,^{1,2} H Okuyama,¹ K Miyamoto,³ T Okuda,³ A Kimura,⁴ H Namatame,³ M Taniguchi,^{3,4} T Aruga¹

¹Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto, Japan; ²JST CREST, Saitama, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ⁴Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan

A large Rashba spin splitting of a metallic surface-state band on a semiconductor surface allows us to open a novel physics such as a spin transport/accumulation at surface. The Rashba spin-split bands on semiconductor surfaces have been identified on Si(111) and Ge(111) surfaces[1-3]. However, there are no metallic surface-state bands for these surfaces and hence cannot contribute to the transport of spins. In the present study, we report on the Rashba spin splitting of a Ge(111) surface covered with a lead monolayer at a coverage of 4/3 [Pb/Ge(111)-β]. From angle-resolved photoelectron spectroscopy (ARPES), we found that one of the surface-state bands for Pb/Ge(111)-β crosses the Fermi level and splits into two. The splitting is due to a surface Rashba effect, which was characterized by spin-resolved ARPES. The surface-state band exhibits a spin splitting of 200 meV and an effective mass of 0.028 m_e at the Fermi level. This implies that the Pb/Ge(111)-β surface can become an ideal prototype for the surface spin transport study. Charge density analysis of the surface state indicates that the large Rashba spin splitting is induced by the asymmetric charge distribution in close proximity to the nuclei of the Pb atoms.

1. I. Gierz *et al.*, Phys. Rev. Lett. **103**, 046803 (2009). 2. S. Hatta *et al.*, Phys. Rev. B **80**, 113309 (2009). 3. K. Sakamoto *et al.*, Phys. Rev. Lett. **103**, 156801 (2009).

2P024

Chemical characterization of SiO₂/SiC interface after nitridation treatment

Y Hu,¹ H Piao,² J Fronheiser,² K Matocha,² A Chatterjee³

¹Canadian Light Source, Saskatoon/SK, Canada; ²General Electric, Niskayuna/NY, United States; ³General Electric, Bangalore, India

Silicon carbide (SiC) has received considerable attention for its potential use in high-power devices. The growth of high quality SiO₂ on SiC is a crucial step to realize these applications. The nitridation of SiO₂/SiC interfaces shows great promise as a means of achieving high quality gate oxides for SiC MOSFET structures. In this work, the SiO₂/SiC structure was prepared by direct oxidation in NO₂, following a NO post-annealing. X-ray absorption spectroscopy (XAS) of Si L- and K-edges, recorded in the surface sensitive TEY, and the bulk sensitive fluorescence yield, together with XPS and SIMS have been used to investigate a series of nitridized SiO₂/SiC interfaces. The results show the formation of SiN at the SiO₂/SiC interface after nitridation treatment. Oxygen has also been incorporated into the oxynitride structure. Great sensitivity of XAS in probing Si, SiC, SiO₂ and SiN_x at different depths is also demonstrated.

2P025

Hole injection enhancement for inverted organic light-emitting devices using tungsten oxide interlayer

YH Kim,^{1,2} S Kwon,³ SM Park,¹ JW Kim^{1,2}

¹Korea Research Institute of Standards and Science, Daejeon, Republic of Korea; ²Department of Nano Science, University of Science and Technology, Daejeon, Republic of Korea;

³Department of Materials chemistry, Sejong Campus, Korea University, Chochiwon, Chung-nam, Republic of Korea

In accordance with emerging new technologies in organic light-emitting diodes (OLEDs), enhancement of light efficiency and extension of application fields are required. Particularly inverted structures, in which electron injection occurs at bottom and hole injection on top, are advantageous due to their easy integration with Si-based driving circuits for active matrix OLED as well as large open area for brighter illumination. In order to get better performance and process reliability, a proper buffer layer for carrier injection is needed. As a buffer material, a few kinds of transition metal oxides for inverted OLED applications have been successfully utilized aiming at efficient hole injection properties. Among them, we chose 2 nm of WO₃ between NPB [N,N'-bis(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine] and Au (or Al) films. The interfacial energy-level alignment and chemical reaction as a function of film coverage have been measured by using in-situ ultraviolet and X-ray photoelectron spectroscopy. The WO₃ interlayer substantially reduces the hole injection barrier irrespective of the kind of electrode metals. From current-voltage and luminescence-voltage measurements for devices fabricated with and without WO₃ interlayer, it turned out that the current efficiency and turn-on voltage are remarkably improved. This observation clearly validates the use of WO₃ interlayer as hole injection for inverted OLED applications.

2P026

Negative contrast photoelectron diffraction replica in secondary electron angular distribution

F Matsui,¹ M Hashimoto,¹ T Matsushita,² N Maejima,¹ H Matsui,¹ K Goto,¹ Y Kato,² H Daimon¹

¹Materials Science, Nara Institute of Science and Technology, Ikoma, Nara, Japan; ²JASRI/SPring-8, Sayo, Hyogo, Japan

Photoelectron diffraction (PD) is an element specific local structure analysis method. Atomic arrangements around photoelectron emitter atom can be deduced from the position of forward focusing peak (FFP) and radii of diffraction rings around them. It was reported that the intensity of FFPs in the inelastic electron angular distribution decreases and PD patterns are destructed due to the defocusing effect by plasmon excitations [J. Osterwalder *et al.* Phys. Rev. B **41**, 12495 (1990), S. Huefner *et al.* Phys. Rev. B **42**, 7350 (1990)]. We have measured 2π -steradian PD and secondary electron patterns from the Ge(111) surface using a display-type analyzer installed at the circularly polarized soft X-ray beamline BL25SU, SPring-8. Kinetic energy of photoelectron was fixed to 600 eV and photon energy was varied. We found that the PD patterns are destructed at 50 eV off from elastic peak. Moreover, the complete replica of negative contrast PD appeared in the secondary electron angular distribution at 200 eV off from elastic peak. The contrast was about one-fourth of that of original PD. The mechanism of this new phenomenon can be understood by the depression of isotropic secondary electron beam intensity by the absorption process of time-reversal PD.

2P027

Atomic structure analysis of silicon oxynitride thin film on 6H-SiC(0001) by two-dimensional photoelectron diffraction

N Maejima,¹ F Matsui,¹ K Goto,¹ N Nishikayama,¹ H Matsui,¹ M Hashimoto,¹ T Matsushita,² Y Kato,² S Tanaka,³ H Daimon¹

¹NAIST, Ikoma, Nara, Japan; ²JASRI/SPring-8, Sayo, Hyogo, Japan; ³Kyushu University, Fukuoka, Fukuoka, Japan

The key issue for the development of SiC-based devices is to reduce the dangling bonds at the SiO/SiC interface which lower the carrier mobility. The epitaxial silicon oxynitride (SiON) thin film newly fabricated by Shirasawa *et al.* is a candidate with high potential for this purpose [1]. They proposed a structure model based on their STM and LEED I-V measurements and suggested that the dangling bonds at the SiO/SiC interface are quenched completely by the replacement of C atoms with N atoms. However, STM is not sensitive to the buried interface and LEED is not an element selective method. We measured N1s and C1s photoelectron diffraction (PD) from SiON thin film at BL25SU, SPring-8. Six bright forward focusing peaks (FFPs) were observed in C1s PD pattern. FFPs indicate the directions of atoms surrounding photoelectron emitter. Three {11-1} and three {110} bright FFPs correspond to the first nearest Si and C atoms, respectively. On the other hand, the FFPs in N1s PD pattern appeared at the mirror symmetric positions of C1s FFPs. This indicates the substitution of C atoms with N atoms and the presence of stacking fault at the interface. Furthermore, we estimated atomic distances between emitter and these neighboring atoms using circular dichroism [2]. We succeeded in the element specific direct atomic structure analysis of the SiON/SiC interface.

[1]T. Shirasawa, *et al.*, PRL **98**, 136105 (2007).[2]H. Daimon, PRL **86**, 2034 (2001)

2P028

Modification of cathode layer and its influence on interfacial energy level and efficiency in polymer solar cells

SM Park,¹ JH Jeon,² OO Park,² JW Kim¹

¹Korea Research Institute of Standards and Science, Daejeon, Republic of Korea; ²Department of Chemical and Biomolecular Engineering Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea

Recent development of organic solar cell approaches the level of 8 % power conversion efficiency by the introduction of new materials, improved material engineering, and more sophisticated device structures. As for interface engineering, various interlayer materials such as LiF, Ca, NaF, and KF have been utilized between Al electrode and active layer. Those materials lower the work function of cathode and interface barrier, protect the active layer, enhance charge collection efficiency, and induce active layer doping. However, the addition of another step of thin layer deposition could be a little complicated. Thus, on a typical solar cell structure of Al/P3HT:PCBM/PEDOT:PSS/ITO glass, we used Li:Al alloy electrode instead of Al to render a simple process. J-V measurement under dark and light illumination on the polymer solar cell using Li:Al cathode shows the improvement in electric properties such as decrease in leakage current and series resistance, and increase in circuit current density. This effective charge collection and electron transport correspond to lowered energy barrier for electron transport at the interface, which is measured by ultraviolet photoelectron spectroscopy. Indeed, through the measurement of secondary ion mass spectroscopy, the Li atoms turn out to be located mainly at the interface between polymer and Al metal. In addition, the chemical reaction between polymer and metal electrodes are measured by X-ray photoelectron spectroscopy.

2P029

2-butyne on Si(001)-2x1 at room temperature: a XPS and NEXAFS studyF Bournel,¹ JJ Gallet,¹ F Rochet,¹ M Silly,² F Sirotti,² F Hennies³¹LCPMR (UMR7614), Université P. et M. Curie, Paris 6, Paris, France; ²Synchrotron SOLEIL, Saint Aubin, France; ³Max-lab, Lund, Sweden

The adsorption of simple organic molecules on Si(001) leads generally to a complex situation, multiples adsorption geometries, dissociation... In order to get a self organized organic layer on Si(001) to foresee subsequent reactions to act as a template, the understanding of the reactions mechanisms of very small molecules on this technical surface is still topical. The adsorption study of 2-butyne was already performed by STM and but for very low coverages (0.25 ML) [1]. Recently, we performed valence band spectroscopy and showed that the molecule adapts a di-adsorption geometry leaving a p bond parallel to the surface confirming the low coverage study [2]. Here, to get a definitive view of the adsorption of 2-butyne on Si(001), we performed real time synchrotron induced photoemission on the C1s level to analyse precisely the adsorption mechanisms to saturation coverage and particularly to follow if there are changes during the process. Si2p photoemission results will also be discussed as well as polarized C K-edge NEXAFS spectroscopy which is the unique tool probing the molecular orbital orientation.

[1] K. Ki-Yeo, et al. J. Chem. Phys. 118 (2003) 6083.

[2] F. Bournel, J.-J. Gallet, F. Rochet, J. Fujii, G. Panaccione, Surf. Sci. 601 (2007) 3750.

2P030

Unusually large charge transfer in C₆₀/Cu(111)WW Pai,¹ HT Jeng,^{2,3} CM Cheng,⁴ CH Lin,¹ XD Xiao,⁵ AD Zhao,⁵ XQ Zhang,⁵ X Geng,⁶ XQ Shi,⁶ MA Van Hove,⁶ CS Hsue,³ KD Tsuei^{3,4}¹Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan; ²Institute of Physics, Academia Sinica, Taipei, Taiwan; ³Department of Physics, National Tsing Hua University, Hsinchu, Taiwan; ⁴National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ⁵Department of Physics, Hong Kong University of Science and Technology, Hong Kong, Hong Kong; ⁶Department of Physics, City University of Hong Kong, Hong Kong, Hong Kong

We present a combined study on C₆₀/Cu(111) by high resolution ARPES/AIPES, STM/STS, LEED-IV and *ab initio* calculations to unravel a long standing issue of the amount of charge transfer in controversy among various experiments and calculations. We find the charge transfer is nearly "optimal", i.e., 3 electrons transferred to LUMO becoming C₆₀³⁻, required for bulk superconductivity in alkali doped compounds. We attribute this unusually large charge transfer without foreign dopants to the substrate reconstruction of [4x4] 7-atom vacancy holes at the interface. ARPES reveals three Fermi surfaces, one electron-like centered at the $\bar{\Gamma}$ -point and two hole-like around the K-point. The total electron occupation is about three. This is confirmed by AIPES; the intensity at the Fermi energy reaches the maximum with only 0.1 K atoms per C₆₀ molecule doped. An STS study finds the LUMO peak is well above the Fermi energy on unreconstructed surface, indicating minimal charge transfer, while it is almost centered at the Fermi energy, suggesting half-filled, in agreement with the PES observations. The reconstructed surface is determined by STM to have 7 Cu atoms removed from the first layer for one C₆₀ molecule to reside. *Ab initio* calculations based on two models find indeed reconstruction lowers the total energy, and confirm the LUMO positions to be consistent with PE and STS measurements. This vacancy model is further checked by LEED-IV analysis to be the most likely interface model. No 2D superconductivity was found at 5 K by STS. Our finding indicates that the interface structure can be important in molecule-electrode contact in molecular electronics. Part of work appears at W.W. Pai *et al.*, Phys. Rev. Lett. **104**, 036103 (2010).

2P031

Characterization of organic surface contamination during semiconductor manufacturing processing by NEXAFS spectroscopyM Müller,¹ B Beckhoff,¹ G Borionetti,² G Bedana,² G Guerinoni,² A Nutsch,³ A Leibold,³ M Otto,³ L Frey³¹Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany; ²MEMC Electronic Materials SpA, Novara, Italy; ³Fraunhofer IISB, Erlangen, Germany

Organic contamination on wafer surfaces with relevance for nanotechnologies and advanced microelectronics gets crucial as the continuously shrinking feature sizes get comparable to the dimensions of clusters and molecules. Especially the manufacturing of highly integrated circuits requires clean surfaces as processes might cause defects involving light elements (e.g. C, N, O, F). Yield issues are observed e.g. due to change of gated oxide integrity by defects, thickness and degradation. Different sources for organic contamination were identified. The environment used for fabrication of microelectronics shows various sources for volatile organic compounds (VOC). The sources for VOCs are packaging materials and carriers or out-gassing and residues of resist layers from lithography. Especially in lithography, non volatile residues remaining on the wafer surface became crucial for subsequent process steps. Silicon wafers from different steps during wafer manufacturing were studied using Near Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS) in Total reflection X-ray Fluorescence (TXRF) mode and Thermo Desorption Gas Chromatography Mass Spectrometry (TD GCMS). The TXRF employing synchrotron radiation in the soft X-ray range provides very low detection limits, which allows for a reliable detection of ultra-trace contaminations of light elements on wafer surfaces. Final cleaning and packaging were identified as areas where detectable organic contamination was transferred to the wafer surface. The application of TXRF-NEXAFS profits from multi-criteria evaluation of the spectra and the study of reference samples matched with TD GCMS.

2P032

Origin of high-mobility in solvent-vapor annealed anthradithiophene derivativeCH Wang,¹ YC Cheng,² JW Su,² LJ Fan,¹ PY Huang,³ MC Chen,³ YW Yang^{1,2}¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Dept. of Chemistry, National Tsing-Hua Univ., Hsinchu, Taiwan; ³Dept. of Chemistry, National Central Univ., Jhongli, Taiwan

Solvent-vapor annealing was used to increase the field effect mobility of soluble triethylsilyl ethynyl anthradithiophene spin-coated on organosilane-terminated silicon dioxide, yielding a high value of $1.2 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$. The cause of improvement was investigated by Atomic Force Microscopy, X-ray Diffraction, and Near-Edge X-ray Absorption Fine Structure spectroscopy. Vapor annealing exerts little effect on the molecular tilt and the crystallinity normal to the surface, but improves the film morphology significantly, presumably yielding better in-plane crystallinity.

2P033

Adsorption of pyridine on Si(001)-2x1 surface revisited by theoretical simulation of XPS, polarization-dependent NEXAFS and HREELS spectraR Coustel,¹ S Carniato,¹ F Rochet¹¹LCPMR, Université Pierre et Marie Curie, Paris, France

The chemical deposition of pyridine on Si(001)-2x1 surface at room temperature is elucidated by confronting the outputs of density functional theory (DFT) theoretical calculations of ground and core-excited states to a body of experimental data encompassing X-ray photoelectron spectroscopy (XPS) and near-edge absorption fine structure spectroscopy (NEXAFS) and high resolution electron energy loss spectroscopy (HREELS). The N 1s ionization potential calculations point to two distinct energy domains, the datively bonded pyridine binding energy being shifted by +3.5 eV from that of the di-sigma and the tetra-sigma geometries, that thus cannot be distinguished one from another. On the other hand, thanks to angular dependent NEXAFS spectroscopy (using linearly polarized radiation) and N1s/C1s core-excited states DFT calculations, the presence of end-bridge and cross-trench butterfly adspecies is demonstrated at room temperature, besides that of dative and tetra-sigma species formed at low temperature. The complementarity and consistency of core-electron spectroscopy data with those of vibrational data is also emphasized.

2P034

H-induced metallization of single crystal ZnO: dependence on the atomic composition of the substrate surfaceK Ozawa,¹ K Mase²¹Department of Chemistry and Materials Science, Tokyo Institute of Technology, Tokyo, Japan; ²Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Japan

Several semiconductor surfaces are known to become metallic by H adsorption. One of these examples is ZnO. Recent studies by Woll and coworkers have revealed that the ZnO(10-10) surface exhibits a metallic character when the surface is covered with H at room temperature and above [1]. Our angle-resolved photoelectron spectroscopy (ARPES) study has identified a single band as an origin of surface metallization [2]. In the present study, we have investigated the electronic structures of the O-terminated ZnO(000-1) and Zn-terminated ZnO(0001) surfaces by ARPES and examined how the surface atomic composition affects the H-induced change of the electronic structure. The measurements were carried out at beam line 11D of the Photon Factory, Japan. H adsorption on the O-terminate surface induces a state just below the Fermi level. The state forms a band crossing the Fermi level. Thus, the (000-1) surface turns to be metallic upon H adsorption. The metallic band shows a parabolically dispersing feature with the Zn 4s character. Moreover, emission intensity of this band is gradually attenuated with increasing H dosage. These features resemble those of the band on the H/ZnO(10-10) surface. Therefore, H-induced metallization should proceed via the same mechanism on both (10-10) and (000-1) surfaces. On the other hand, the Zn-terminated surface remains to be a semiconductor even after H adsorption. This is due to a high etching rate of the surface Zn atoms by H atoms in comparison with other two surfaces.

[1] Ch. Woll, Prog. Surf. Sci. 82, 55 (2007). [2] K. Ozawa and K. Mase, Phys. Stat. Sol. A, 207, 277 (2010).

2P036

Depth resolved electronic structure of an LSMO/STO superlattice via standing-wave excited angle-resolved photoemission

AX Gray,^{1,2} C Papp,^{2,3} B Balke,^{2,4} S H Yang,⁵ M Huijben,⁶ E Rotenberg,⁷ A Bostwick,⁷ S Ueda,⁸ EM Gullikson,⁷ JB Kortright,² FMF De Groot,⁹ K Kobayashi,⁸ CS Fadley^{1,2}

¹Physics Department, University of California, Davis, CA, United States; ²Materials Sciences Division, LBNL, Berkeley, CA, United States; ³Physical Chemistry II, University of Erlangen, Erlangen, Germany; ⁴Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität, Mainz, Germany; ⁵IBM Almaden Research Center, San Jose, CA, United States; ⁶Faculty of Science and Technology, MESA Institute for Nanotechnology, University of Twente, Enschede, Netherlands; ⁷Advanced Light Source, LBNL, Berkeley, CA, United States; ⁸National Institute for Materials Science, SPring-8, Hyogo, Japan; ⁹Department of Chemistry, Utrecht University, Utrecht, Netherlands

We have determined the depth-resolved composition profiles and electronic structure of a SrTiO₃/La_{0.67}Sr_{0.33}MnO₃ superlattice via standing-wave excited angle-resolved soft and hard X-ray photoemission. The epitaxial superlattice samples consisted of 48 and 120 bilayers of cubic colossal magnetoresistive LSMO (15.5 Å), and paramagnetic STO (15.6 Å). These were studied using excitation energies of 833.2 eV at ALS, and at 5,946 eV at Spring-8. Analyzing rocking curves at both energies permits determining depth-resolved composition profiles and optical constants. Soft X-ray ARPES also shows distinctly different *k*-space maps of Mn 3d e_g and t_{2g} states from the bulk-like and interface-like regions of the LSMO. Additionally, a shift was observed in the position of the Mn 3p photoemission peak which is not found for the peaks in any other element; this suggests a change in the Mn chemical and magnetic state near the STO/LSMO interface, consistent with crystal-field distortion effect. Funded by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

2P037

Surface states on heavy rare earth metals

S Gorovikov¹

¹Canadian Light Source Inc., Saskatoon, SK, Canada

High resolution angle-resolved photoemission spectroscopy (ARPES) has been employed to study of the electronic structure and dynamics of *d*-like surface states at heavy rare-earth metals from Gadolinium to Holmium. ARPES is a powerful tool for studying of interaction of conduction electrons with low-energy collective excitations in solids such as phonons and magnons. The technique is capable to reveal momentum- and energy-dependent quasiparticle dynamics in order to establish the quantitative link between the microscopic electronic structure and macroscopic transport phenomena in solids. Most of experimental and theoretical efforts spent so far have been focused on surfaces of noble metals. Much less is known on the electron dynamics at surfaces of the lanthanides, especially ferromagnetic ones. Electron coupling to both lattice and spin waves is expected to be an equally important. The lanthanides chosen for the investigation have very different magnetic phase diagram while exhibit rather similar electronic structure and dynamics of the lattice. Therefore thorough analysis of the temperature-dependent broadening of the surface states provides a unique opportunity to distinguish between electron-phonon and electron-magnon scattering contribution into the lifetime of the photohole.

2P038

Orbital and charge configuration in LaNiO₃-LaAlO₃ superlattices studied by X-ray resonant reflectivity

E Benckiser,¹ M Haverkort,¹ S Brück,^{2,3} E Goering,² HU Habermeier,¹ V Hinkov,¹ B Keimer¹

¹Max Planck Institute for Solid State Research, Stuttgart, Germany; ²Max Planck Institute for Metal Research, Stuttgart, Germany; ³Experimentelle Physik 4, Physikalisches Institut, Würzburg, Germany

Motivated by the theoretical prediction of high-temperature superconductivity [1,2], we started to investigate nickelate superlattices. To study the interfacial orbital and electronic configuration and the effect of strain in nickelate superlattices we performed resonant soft X-ray absorption and reflectometry experiments at BESSY II (Berlin, Germany), using the advanced 3-axis UHV reflectometer described in Ref. [3]. We focused on a LaNiO₃-LaAlO₃ superlattice grown on different strain-inducing substrates. We measured reflectivity in specular geometry, i.e. the momentum transfer was always parallel to the surface normal *z*. By using soft X-rays with energies close to the Ni L edge, we investigated a possible orbital, spin, and charge modulation of the Ni ions along *z*. We present fits to the reflectivity, which allow us to compare our experimental data for energy scans at constant momentum transfer (const. *q_z*) scans with simulations. We will discuss that the small linear dichroism observed in the Ni L edge XAS spectrum is enhanced in the const. *q_z* scans at the {002} superlattice peak reflecting a modulation in the population of *x*²-*y*² and *3z*²-*r*² bands in the LaNiO₃ layers along *z*.

[1] J. Chaloupka and G. Khaliullin, PRL **100**, 016404 (2008), [2] P. Hansmann et al., PRL **103**, 016401 (2009), [3] S. Brück et al., Rev. Sci. Instrum. **79**, 083109 (2008)

2P039

Microscopic origin of paraelectric phase transition in BaTiO₃ probed by resonant X-ray emission spectroscopy

Y Isohama,¹ N Nakajima,¹ H Maruyama,¹ Y Tezuka,² T Iwazumi³

¹Grad. Sch. of Sci., Hiroshima Univ., Higashi-Hiroshima, Japan; ²Grad. Sch. of Sci. Tech., Hirosaki Univ., Hirosaki, Japan; ³Grad. Sch. of Engrn. Osaka Prefecture Univ., Sakai, Osaka, Japan

Perovskite BaTiO₃ (BTO) is a typical material of displacive-type ferroelectric and undergoes paraelectric phase transition at Curie temperature $T_c=120$ °C. The dielectric polarization below T_c has been explained by an off-centered Ti⁴⁺ ion in distorted TiO₆ polyhedron. Recently, critical slowing down has been observed in the polarization clusters using a pulsed X-ray laser (PXL) technique [1], and it has been concluded that fluctuation time of the clusters takes a maximum value at 4.5 °C above T_c , which invokes a discussion on the possibility of order-disorder type transition from a microscopic point of view. This fact prompts us to get the information about locally polarized state in ferroelectric around T_c . For this purpose, resonant X-ray emission (RXE) spectroscopy is an effective technique, because the emission is caused by the interaction of X-ray with matter localized around the absorbing atom. Ti K RXE spectra of in BTO powders were measured from room temperature up to 200 °C on BL-7C at KEK-PF. Two Raman peaks have been observed and show the different behaviors; the one remains even above T_c , the other disappears at several °C above T_c . It is noted that these Raman peaks are associated with charge transfer (CT) excitations from oxygen to Ti, so that the two CT peaks reveal inversion-symmetry breaking around Ti site. The present results suggest the local polarization remains up to several °C higher than T_c . The higher transition temperature in microscopic region, deduced from our RXE spectra as well as a PXL technique, provides us an intrinsic aspect of precursory phenomena in ferroelectrics.

[1] K. Namikawa *et al.*, Phys. Rev. Lett. **103**, 197401 (2009).

2P040

Resonant Raman scattering of polarized and unpolarized X-ray radiation from Mg, Al and Si

D Sokaras,¹ M Müller,² M Kolbe,² B Beckhoff,² C Zarkadas,^{1,3} AG Karydas^{1,4}

¹Institute of Nuclear Physics, N.C.S.R. "Demokritos", Athens, Greece; ²Physikalisch-Technische Bundesanstalt (PTB), Berlin, 10587, Germany; ³PANalytical B.V., Almelo, Netherlands; ⁴Nuclear Spectrometry and Applications Laboratory, International Atomic Energy Agency (IAEA), Seibersdorf, Austria

The X-ray resonant Raman scattering (RRS) effect of polarized and unpolarized radiation is investigated in the vicinity of the 1s absorption threshold of low Z elements like magnesium, aluminum and silicon. For the polarized and tunable exciting X-ray radiation the plane grating monochromator (PGM) beam line at the PTB laboratory in BESSY II synchrotron radiation facility was employed, while unpolarized X-ray beams were induced by 1 MeV proton beam irradiation on various pure thick targets. For the latter case, a novel proton induced XRF scattering chamber was designed and installed at the Tandem accelerator laboratory of Institute of Nuclear Physics at N.C.S.R. "Demokritos". The total RRS cross sections deduced from both independent excitation modes were found in a good agreement, within the experimental uncertainties. Further on, calculations based on existing theoretical models were performed in order to evaluate the dependence of the RRS to the incident beam polarization state as well as the absolute value of the total RRS cross sections, where systematic differences were obtained.

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2P041

dd and magnetic excitations in layered cuprates seen by high resolution Cu L₃ edge RIXS

M Moretti Sala,¹ V Bisogni,² LJP Ament,³ L Braicovich,¹ C Aruta,⁴ G Balestrino,⁵ H Berger,⁶ N B Brookes,² M Grioni,⁶ M Guarise,⁶ PG Medaglia,⁵ F Miletto-Granozio,⁴ M Minola,¹ M Salluzzo,⁴ GM De Luca,⁴ T Schmitt,⁷ J van den Brink,⁸ G Ghiringhelli¹

¹CNR-SPIN/IOM and Dip. di Fisica, Politecnico di Milano, Milano, Italy; ²ESRF, Grenoble, France; ³Institute-Lorentz for Theoretical Physics, Universiteit Leiden, Leiden, Netherlands; ⁴CNR-SPIN and Dip. di Scienze Fisiche, Università Federico II, Napoli, Italy; ⁵CNR-SPIN and Dip. di Ingegneria Meccanica, Università Tor Vergata, Roma, Italy; ⁶Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland; ⁷SLS-PSI, Villigen, Switzerland; ⁸Leibniz-Institute for Solid State and Materials Research, Dresden, Germany

Resonant Inelastic X-ray Scattering (RIXS) is a powerful tool for measuring neutral excitations in strongly correlated systems. Using the high resolution AXES (at ID08-ESRF) and the SAXES (at ADDRESS-SLS) spectrometers at the Cu L₃ edge we have observed magnetic excitations in cuprates [PRL102,167401]. Recently we have demonstrated both theoretically [PRL103,117003] and experimentally [PRL104,077002] that single magnons can be probed by the RIXS process. Moreover their dispersion could be observed for the first time in the antiferromagnetic compounds La₂CuO₄. An important ingredient of the theory presented is an atomic model which allows us to infer the single magnon cross section. The same model was also applied to the fitting of dd excitations in this and other compounds to determine the symmetry and energy position of the ligand field split 3d states of Cu ions. It also turns out that RIXS cross sections reasonably agree with the experimental data.

2P042

The duality of charge carriers in LaAlO₃/SrTiO₃ superlattices revealed by Resonant Inelastic X-ray Scattering

K Zhou,¹ M Radovic,² J Schlappa,¹ V Strocov,¹ J Mesot,³ L Patthey,¹ T Schmitt¹¹Paul Scherrer Institut, Swiss Light Source, Villigen - PSI, Switzerland; ²Laboratory for synchrotron and neutron spectroscopy, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; ³Paul Scherrer Institut, ETH- Zurich and EPFL-Lausanne, Switzerland

Oxide heterostructures have been attracting great attention due to extraordinary phenomena occurring at the interface and their potential application for device design employing oxide materials. A particularly fascinating system is the two-dimensional conductive interface between the band insulators LaAlO₃ and SrTiO₃ which can be even driven to magnetic and superconducting phase at low temperatures. Resonant inelastic X-ray scattering at Ti L-edges is particularly suitable to address the electronic structure of its interface since the signature of conducting Ti³⁺ states clearly displays a strong dd excitation while Ti⁴⁺ states exhibit no excitations in the low energy loss regime. Our studies on [(LAO)_m/(STO)₁₀]₁₀ superlattices prepared by pulsed laser deposition unambiguously reveal two types of carriers giving rise to localized and delocalized Ti 3d bands, respectively. The dual character of these carriers is even preserved after annealing under O₂ atmosphere and high temperature. Varying the number of LAO unit cells *m* showed that oxygen vacancies contributed carriers enhance for larger *m* but saturate at a certain value. Increasing *m*, the electron transfer conduction mechanism begins to set in compensating the electric potential and keeping the whole system well in balance.

2P043

Polarization-dependent Ti K X-ray absorption and emission studies of Ti₂O₃ single crystal

H Sato,¹ H Maso,² Y Utsumi,² H Kurihara,² Y Mukaegawa,² Y Tezuka,³ T Iwazumi,⁴ F Iga,^{5,6} M Tsubota,⁵ H Namatame,¹ M Taniguchi^{1,2}¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ³Graduate School of Science and Engineering, Hirosaki University, Hirosaki, Japan; ⁴Graduate School of Science, Osaka Prefecture University, Sakai, Japan; ⁵ADSM, Hiroshima University, Higashi-Hiroshima, Japan; ⁶IAMR, Hiroshima University, Higashi-Hiroshima, Japan

Ti₂O₃ exhibits metal [high-temperature side] - insulator [low-temperature side] transition (MIT) around 450 K. Recently, we have revealed the large Ti 3d configuration change due to MIT by the Ti L absorption spectroscopy [1] and anisotropy of the electronic structure reduces in the metallic phase. In this study, we present the polarization-dependent Ti K X-ray absorption and emission (XAS and XES) spectra of Ti₂O₃ single crystal measured at BL-7C and BL-15B1 at KEK-PF. Both the XAS and XES spectra show the difference between *E*//*c* and *E*⊥*c*-cases, where the *c*-axis is parallel to the Ti ion pair direction. The main peak of the *E*//*c*-spectrum is 3 eV lower than the *E*⊥*c*-spectrum at 300 K, reflecting the anisotropic Ti 4p unoccupied states, and the energy separation decreases to 2 eV at 520 K in consistent with reduction of anisotropy. The Raman features in the Ti K_α XES spectra taken far below the Ti K edge are very similar to the XAS feature including the polarization dependence, suggesting that the Raman features originate from the 2p-4p monopole transition as TiO₂ [2].

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2P044

Theory of resonant X-ray scattering by magnetic excitations

MW Haverkort¹¹Max-Planck Institute for Solid State Research, Stuttgart, Germany

It has been long recognized that Resonant elastic X-ray Diffraction (RXD) at the Transition Metal L_{2,3} edge is a very sensitive tool to measure magnetic ordering. The resonant enhancement of the scattering form factor is, by the optical theorem, related to the X-ray absorption spectral (XAS) function. The energy dependence can, due to the strong excitonic character of the intermediate state, be calculated relatively accurately with the use of local cluster calculations. Polarization and azimuthal dependence is given by the simple relation that the scattering cross section is (in spherical symmetry) proportional to: $F(0) \{ \text{ein} \cdot \text{eout}^* \} + F(1) \{ \text{ein} \cdot \text{eout}^* \cdot m \} + F(2) \{ (\text{eout}^* \cdot m) \{ \text{ein} \cdot m \} - 1/3 \{ \text{ein} \cdot \text{eout}^* \} \}$ [1]. Within this talk I will first show how these relations change when one includes the crystal symmetry. In several cases this leads to very large changes [2]. Secondly I will show how these relations can be extended to not only describe the elastic scattering, but also the inelastic diffraction. I will present a tractable theory for the Resonant Inelastic X-ray Scattering (RIXS) spectral function of magnons. The low-energy transition operator is written as a product of local spin operators times fundamental XAS spectra. This leads to simple selection rules for the magnetic cross section and to a common description for XAS, RXD and RIXS [3].

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2P045

X-ray absorption edge of graphite evaluated from the resonance inelastic X-ray scattering and X-ray Raman scattering

Y Muramatsu,¹ W Yang,² J Denlinger,² E Gullikson²

¹University of Hyogo, Himeji, Hyogo, Japan; ²Lawrence Berkeley National Laboratory, Berkeley, CA, United States

X-ray emission spectral profile depends on the excitation energy. Especially in the excitation near the X-ray absorption threshold, the X-ray emission profiles drastically change from the X-ray fluorescence (XRF). Such the resonance inelastic X-ray emission scattering (RIXS) has been a novel probe for the electronic structure analysis of advanced materials. Additionally in the lower-energy excitation from the threshold, X-ray Raman scattering can be often observed. Consequently, we could obtain the fine information of X-ray absorption edge structure from the XRF, RIXS, and X-ray Raman scattering [1]. To demonstrate the relationship between the X-ray absorption edge structure and X-ray emission spectra, we have finely measured the XRF, RIXS, and X-ray Raman scattering of the highly oriented pyrolytic graphite (HOPG). X-ray emission spectral measurements were performed at the beamline BL-8.0.1 and X-ray absorption measurements at BL-8.0.1 and BL-6.3.2 in the Advanced Light Source (ALS). The X-ray absorption edge of HOPG was evaluated at 284 eV from the border between RIXS and X-ray Raman scattering.

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2P046

Characterization of 1s core-excited states of Cl containing molecules by frequency detuned resonant inelastic X-ray scattering

M Kavčič,¹ M Žitnik,¹ K Bučar,¹ S Carniato,² L Journal,² R Guillemin,² M Simon²

¹J. Stefan Institute, Ljubljana, Slovenia; ²Laboratoire de Chimie Physique-Matière et Rayonnement, UMR 7614, Paris Cedex, France

We have studied electronic state interference and nuclear dynamics after 1s shell excitation of HCl, CH₃Cl and Cl₂ molecules by observing the resonant inelastic X-ray scattering (RIXS) around the chlorine 1s edge. A Johansson type crystal spectrometer of J. Stefan Institute [1] was coupled to the ID26 beamline at ESRF synchrotron in order to record a comprehensive series of high resolution KL and KV RIXS spectra. A broad range of the near-threshold excitation energies was covered to include the region of dissociative 1s⁻¹s* resonance as well as the higher lying Rydberg states converging to Cl[1s] threshold. While spectral lines corresponding to excitations into bound Rydberg states exhibit a well-known linear dispersion, a complete breakdown of linear dispersion law is observed for the 1s⁻¹σ* core-excited molecular state revealing a characteristic interplay between the fast dissociation and the radiative relaxation. This characteristic behavior can be described qualitatively using the concept of the effective duration time of the RIXS process [2]. An exact theoretical description is provided by RIXS formalism for electronic transitions between parallel potential energy curves of the intermediate and final states [3]. The extensive calculations for HCl molecule based on *ab initio* calculated potential energy curves are presented in excellent agreement with the experimental data. Strong interference effects have been evinced in the region between the main resonances resulting from the coherent excitation to σ* and Rydberg states.

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2P047

Elastic and resonant X-ray Raman scattering in the K-shell energy region of HCl

S Carniato,¹ P Selles,¹ L Journal,¹ R Guillemin,¹ F Gel'mukhanov,¹ M Simon²

¹Laboratoire de Chimie-Physique Matière et Rayonnement (LCPMR), UMR 7614 du CNRS, Université Pierre et Marie CURIE (Paris VI), Paris, France; ²Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden

Resonant elastic and inelastic X-ray Raman scattering (RXS, RIXS) in the 2-10 keV range of isolated atoms and molecules has recently experienced growing interest [1-5]. As shown in the case of core-excited chlorinated molecules (HCl, CF₃Cl), RIXS measurements in this range take advantage of ultrafast nuclear dynamics and high-energy-resolution decay spectra, taken with long-pulse light sources. We analyze here the interplay (interference process) between the elastic (Thomson scattering) and the Resonant elastic X-ray scattering that has been observed after resonant K-shell excitation in HCl. Following a combined experimental and theoretical analysis we interpret the complex shape evolution of the spectra as a function of the excitation (detuning) energy and we will discuss the role of nuclear motion using the concept of effective duration time of the scattering process [6-7].

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2P048

Detailed measurement of Ti 2p resonant X-ray Raman scattering of TiO₂ and its polarization dependence measurements

Y Tezuka,¹ S Nakagawa,¹ T Shinoya,¹ H Soyama,¹ N Nakajima,² O Morimoto³

¹Graduate School of Science and Technology, Hirosaki University, Hirosaki, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan

Resonant X-ray Raman scattering (RXRS) spectra of rutile (TiO₂) were observed under excitation at around the Ti 2p absorption edge. The XRS measurements were performed at the beam-line BL2C in Photon Factory, KEK. The X-ray emission spectrometer was improved recently so that beamline monochromator and undulator gap can be controlled by same computer. Thus, a numbers of emission spectra can be observed continuously. The excitation energy was changed fine step (~0.3 eV) from 455 to 485 eV. About one hundred numbers of spectra were plotted in a graph as intensity plot. Detailed change of emission spectra, which include fluorescence and Raman scattering spectra, at the resonance could be made clear. Polarization dependence of the RXRS was also observed. In addition, partial fluorescence yield (PFY) spectrum, which is observed emission intensity around Ti 3d → 2p fluorescence energy with about 50 eV band width, was observed. The PFY spectrum shows clear polarization dependence in the charge transfer (CT) satellite region, suggesting the Raman scattering of CT excitation has clear selection rules.

2P049

Change of electronic structure at the ferroelectric phase transition of BaTiO₃ measured by X-ray Raman scattering

Y Tezuka,¹ S Nakagawa,¹ T Shinoya,¹ H Soyama,¹ N Nakajima,² H Osawa,³ S Nozawa,⁴ T Iwazumi⁵

¹Graduate School of Science and Technology, Hirosaki University, Hirosaki, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ³JASRI/SPRING-8, Sayo-cho, Sayo-gun, Hyogo, Japan; ⁴Photon Factory, Institute of Materials Structure Science, Tsukuba, Japan; ⁵Graduate School of Engineering, Osaka Prefecture University, Sakai, Japan

X-ray Raman scattering (XRS) spectra of ferroelectric BaTiO₃ were observed under excitation at around the Ti 1s absorption edge. X-ray emission spectra around Ti Kα fluorescence energy were observed. BaTiO₃ undergoes ferroelectric phase transition at about 120°C from tetragonal ferroelectric phase to cubic paraelectric phase. The mechanism of the phase transition is still under discussion, because the hybridization between Ti and O affect strongly to it [1]. Though the study of electronic structure is necessary, it could not be performed sufficiently because the sample is an insulator. In this study, unoccupied Ti 3d state was observed by XRS of Ti 2p3d excitation, where underline denotes core hole. The Ti 3d state shows anisotropy concerning to the spontaneous polarization direction and change when the BaTiO₃ undergoes phase transition. The results reveal the effect of the hybridization to the ferroelectric phase transition. [1] R.E. Cohen, Nature 358, 136 (1992).

2P050

The sub-bandgap energy loss satellites in Be 1s RIXS spectra in beryllium compounds

I Kuusik,¹ T Käãmbre,¹ K Kooser,^{1,2} V Pustarov,³ V Ivanov,³ E Kukk,² A Kikas¹

¹Institute of Physics, University of Tartu, Tartu, Estonia; ²Department of Physics and Astronomy, Turku, Finland; ³Ural State Technical University-UPI, Yekaterinburg, Russian Federation

Resonant X-ray inelastic scattering spectra have been measured in BeO, phenakite and chrysoberyl crystals with the excitation energy near the beryllium K edge. The experiments were performed at beamline I511-3 in MAX-lab, Sweden. The experimental RIXS spectra excited in the vicinity of the core resonance show two principal features: the scattering on a valence exciton (this band verges into the characteristic Kα emission at higher excitation energies), and a remarkably strong energy loss side-band (more than 6 eV wide) to the elastic scattering peak. This sideband is present in spectra of all studied compounds, but its strength and shape vary strongly. This side-band arises from the so-called participator emission where the core photoexcited electron participates in a radiative transition to fill the core hole losing some energy in the process. To gain further insight to this process, electronic transitions in a system with a single symmetric vibrational mode have been modelled. The model is based on the Born-Oppenheimer approximation and the Franck-Condon principle for electronic transitions. The shape of the potential energy curves has been described by Morse potentials. The calculated emission spectra are based on the Kramers-Heisenberg formula. The phonon relaxation has been simulated empirically by „smearing“ the photoabsorption-populated vibrational levels with lower levels using an exponential distribution. This simple model is able to qualitatively explain this wide energy loss shoulder, although it has difficulties to explain the variation of this width between different beryllium compounds.

2P051

A Ti 2p RIXS study of Ni, Co and I doped titania filmsT Käämbre,¹ I Kuusik,¹ R Pärna,¹ U Joost,^{1,2} I Kink,^{1,2} V Kisand,^{1,2} E Nõmmiste,¹ A Kikas¹¹Institute of Physics, University of Tartu, Tartu, Estonia; ²Estonian Nanotechnology Competence Center, Tartu, Estonia

The applications of TiO₂ include catalysts and optical coatings. It is widely used in solar cell applications, while its band gap is somewhat too large for best efficiency using direct sunlight. Band gap engineering using substitute metal anions has therefore been attempted [1, 2]. The catalytic properties of titania cause light-induced superhydrophilicity at the surfaces, which makes the surfaces 'self-cleaning'. The thin film samples in our study were spin-coated from the sol-gel precursors, which is a simple and robust method for producing titania films of good quality, while the post-deposition annealing gives good control of crystallite size and crystal structure. The sample sets of pristine and iodine, Ni and Co doped titania annealed at different temperatures were produced and studied. The different X-ray absorption spectral 'fingerprints' [3] of the rutile and anatase phase allowed us to study the dopant effect on the crystal phase transition temperature, while RIXS provides (though not always straightforward) information about the gap states. Ni doped films annealed at moderate (ca 500°C) temperatures were seen to produce best results for application; the details and the development of the series will be discussed.

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2P052

Resonant X-ray emission spectroscopy of 3d metals and oxidesWA Caliebe,¹ E Welter,¹ P Machek²¹DESY, Hamburg, Germany; ²Institute of Physics, Prague, Czech Republic

We measured 1s2p and 1s3p resonant X-ray emission spectroscopy (RXES) spectra of Fe and Cu, and some of their oxides, with the dispersive spectrometer at beamline W1 at the DORIS III storage ring at DESY [1]. The energy resolution of the incident beam was limited by the vertical source size and the Si(111) monochromator, and was set to $2 \cdot 10^{-4}$ as a compromise between energy resolution and intensity. The incident flux was of the order of $5 \cdot 10^{10} - 1 \cdot 10^{11}$ photons/s. The spectra were measured with the most appropriate Si-analyzer for the specific edges in order to optimize the energy resolution. The energy resolution of the spectrometer is of the order of 0.5eV to 1.2eV for different fluorescence lines. We measured the complete RXES spectra, from which we extracted total (TFY) and partial fluorescence yield (PFY) spectra. The PFY-spectra for different fluorescence lines differ slightly in the pre-edge region, which might be attributed to different final-state interactions. Surprisingly, the 1s2p RXES-spectra seem to have sharper features. A detailed data analysis is still under progress [2].

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2P053

Non-resonant inelastic X-ray scattering of cubic BN and AlbiteWA Caliebe,¹ M Wilke²¹DESY, Hamburg, Germany; ²GeoForschungszentrum, Potsdam, Germany

We applied non-resonant inelastic X-ray scattering to measure the B K-edge in cubic BN at 188eV, and the inelastic X-ray spectrum from 0 to 180eV energy transfer. For both samples, we measured the spectra at different scattering angles between 20° and 70°. The energy resolution of the spectrometer was dominated by the energy resolution of the monochromator, which was about 2.5eV (FWHM) at 9.1keV. The incident flux was of the order of $5 \cdot 10^{10}$ photons/s in a beam size of 5mm x 1mm (h x v). The scattering geometry was in the vertical plane. In the case of cubic BN, we could not observe any changes in the position and shape of the edge in our momentum transfer range, which varied between 1.6Å^{-1} and 4.6Å^{-1} . In the case of LiF, significant changes in the line-shape have been observed at the Li and F K-edges [1] in similar momentum transfer range. At higher momentum transfers, monopole transitions have been observed in the case of LiF. The spectra of Albite are dominated at low scattering angles by broad features, which can be attributed to plasmon-like structures, which overlap with the Na L-edges. At higher scattering angles, the Compton-peak is dominating, however, some structure at the low-energy side can be attributed to the Na L-edge. A detailed analysis of the data is still ongoing, and additional experiments are planned for the future.

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2P054

Borrmann spectroscopy - a novel tool for the analysis of quadrupole transitionsM Tolkiehn,¹ SP Collins²¹HASYLAB at DESY, Hamburg, Germany; ²Diamond Light Source Ltd., Chilton, United Kingdom

We will present a novel tool for the investigation of quadrupole absorption features in the X-ray absorption near edge structure (XANES). It is based on the Borrmann effect, which was discovered [1] and described theoretically [2] already half a century ago. Recently it was discovered by Pettifer et al. [3] that the quadrupole absorption is dramatically enhanced in the Borrmann effect. This is caused by the standing wave field, which is formed inside the crystal. For certain reflections the low electrical field intensity at the atoms leads to a low dipole absorption (anomalous transmission). At the same time the high field gradient results in an enhanced quadrupole absorption. Therefore the intensity of the reflected beam strongly depends on the quadrupole absorption cross section of the atoms at the nodes of the standing wave field. This serves as a basis of the novel Borrmann spectroscopy method. By proper choice of Laue reflections the quadrupolar spectral features can be enhanced to such an extent that they dominate the absorption spectrum. We will present the theoretical foundations of this method including its temperature and thickness dependence. Experimental results obtained at different temperatures and sample thickness from Laue reflections of Rutile (TiO₂) at the Ti-K edge will be shown. Furthermore we will show first Borrmann spectroscopy results from doped crystals.

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2P055

Symmetry selective resonant X-ray emission spectroscopy study of tungsten dioxide (WO₂) at the O K-edgeD Cockburn,¹ B Kennedy,¹ JD Denlinger,² F Hennies,³ A Pietzsch,³ RG Egdell,⁴ C McGuinness¹¹School of Physics, Trinity College Dublin, Dublin, Ireland; ²Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States; ³MAXLab, Lund University, Lund, Sweden; ⁴Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, Great Britain

The structure of WO₂, a metallic oxide with a monoclinic unit cell, can be visualised as a rutile-like crystal where the metal-metal bonds along the rutile-like *c*-axis are dimerised similar to the VO₂ monoclinic structure. The inherent structural repeat units of edge-sharing WO₆ octahedra and W₃O planes, a feature of all rutile systems, persists in this monoclinic structure. W₃O planes result in oxygen *sp*² hybridisation, and are parallel with the monoclinic *a*-axis (equivalent to the rutile *c*-axis). We have applied a combination of X-ray absorption spectroscopy (XAS) and resonant X-ray emission spectroscopy (RXES) at the O K edge to a single crystal of WO₂. Like other rutile-like oxides, WO₂ exhibits a linear dichroism (at the O K edge) with respect to the orientation of the linearly polarised synchrotron light and the rutile-like *c* axis. RXES at the O K edge can utilise this linear dichroism to selectively probe the occupied oxygen 2*p* density of states in the valence band. Reported here are a comprehensive set of RXES spectra at the O K edge, measured in both in-plane and out-of plane scattering geometries with two differing incident polarisations.

2P056

HFS Calculation and Computed Lβ₂ satellites spectra of ⁷⁵Re, ⁷⁷Ir and ⁷⁹AuS Poonia¹¹Division of Natural Resources and Environment, Central Arid Zone Research Institute, Jodhpur, Rajasthan, India

The satellite spectra arising due to L₃M_x-M_xN_{4,5} (x = 1-5) transition array in X-ray emission spectra of ⁷⁵Re, ⁷⁷Ir and ⁷⁹Au, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree-Fock-Slater (HFS) data on 1s⁻¹2p¹3x¹ and 2p_{3/2}⁻¹3x¹3x¹ Auger transition energies, their relative intensities have been estimated by considering cross sections of singly ionized 2x¹ (x = s, p) states and then of subsequent Coster-Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in Lβ₂ spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that two satellites observed in the Lβ₂ region of the X-ray spectra of the elements with Z = 75 to 79 named β₂^I and β₂^{II} in order of increasing energy are mainly emitted by L₃M_{4,5}-M_{4,5}N_{4,5} transitions. The satellite β₂^I has been assigned to the superposition of the transitions ³F₄-³G₅ and ³F₄-³D₃, contributing in order of decreasing intensity, and the line β₂^{II} has been assigned to mainly the ¹F₃-¹G₄ and ³P₀-³D₁ transitions. The possible contributions of other transitions of the L₃M_x-M_xN_{4,5} (x = 1-5) array having appreciable intensities have also been discussed.

2P057

Measurements of L_3 -subshell absorption jump ratios and jump factors of Pb, Th and U

KS Kahlon,¹ BS Sidhu,¹ AS Dhaliwal,¹ KS Mann¹

¹Department of Physics, Sant Longowal Institute of Engineering & Technology, Sangrur, Punjab, India

Absorption jump ratios and jump factors are ratios of mass attenuation coefficient or photoelectric absorption coefficient on lower and upper side of absorption edge. Shell-wise photo effect cross sections at the edges can be obtained from the absorption jumps without any theoretical assumptions. This is an elegant method for determining the shell-wise photo effect cross sections at the edges. Keeping this in mind, L_3 -subshell absorption jump ratios and jump factors of Pb, Th and U have been measured by using EDXRF spectroscopy technique. Si (Li) detector with resolution ~ 300 eV (FWHM) at 5.9 keV photon energy and reflection geometry (90°) were used for detecting the emitted fluorescent X-rays from the target excited by ^{241}Am (100 mCi) radioactive point source. Measured values of jump factors and jump ratios of Pb, Th and U are compared with theoretical values obtained from WinXcom programme [Radiation Phys. Chem. 60: 23, 2001]. The experimental results are in agreement with the theoretical values within uncertainties of measurements. The measured values of jump factors and jump ratios are reported for the first time.

2P058

Transmission grating spectrograph with pinhole aperture for soft X-ray spectroscopy of a laser plasma X-ray source

N Yamaguchi,¹ T Sasaya,² H Yokosuka,² S Aoki²

¹Physics Lab., Liberal Arts and Science, Graduate School of Medicine and Pharmaceutical Sciences, Univ. of Toyama, Toyama, Japan; ²Graduate School of Pure and Applied Science, Univ. of Tsukuba, Tsukuba, Japan

In recent years, transmission gratings with high line densities up to 10000 linepairs/mm have been utilized, then spectroscopic measurements can be performed for the shorter wavelength soft X-ray range with enough wavelength resolution. In this work, we have performed spectroscopy of laser plasma with a pinhole transmission grating spectrograph (PTGS) system. The fine grating, spacing d , is fabricated perpendicularly to the supporting stripe which has the larger spacing, d_s , of about $1\ \mu\text{m}$. The diffraction pattern projected by a point X-ray source comes from the two-dimensional Fraunhofer diffraction of the rectangular opening array with a width of d and height of d_s . Therefore, the PTGS system provides the diffraction pattern along the wavelength dispersion (the normal spectrum) and that from the support stripe grating which appears vertically to the normal spectrum. In this system, one can determine wavelengths of observed spectral lines without observing the 0-th order light by using the output spectrum due to the d_s grating. On the other hand, it is necessary to detect spectrum involving the 0-th order light which is used as the origin of the wavelength axis in the conventional slit transmission grating (STGS) system. Spectral images of laser-produced plasma have been observed with the diffraction pattern from the support stripe at the wavelength range around 5 nm. Precise procedures in determining wavelengths of observed spectral lines and results will be presented.

2P059

Recent advances in the determination of atomic parameters for modeling K lines in cosmically abundant elements

P Quinet,^{1,2} P Palmeri,¹ C Mendoza,³ MA Bautista,⁴ J Garcia,^{5,6} MC Witthoef,⁵ TR Kallman⁶

¹Astrophysique et Spectroscopie, Université de Mons - UMONS, Mons, Belgium; ²IPNAS, Université de Liège, Liège, Belgium; ³Centro de Física, IVIC, Caracas, Venezuela; ⁴Department of Physics, Western Michigan University, Kalamazoo, MI, United States; ⁵IACS-Department of Physics, The Catholic University of America, Washington, DC, United States; ⁶NASA Goddard Space Flight Center, Greenbelt, MD, United States

The unprecedented spectral capabilities and sensitivity of recent orbiting X-ray telescopes (*Chandra*, *XMM-Newton*, *Suzaku*) have opened the door for quantitatively accurate studies of atomic inner-shell processes in astrophysical plasmas. This trend will continue to grow with the launch of future instruments such as the *International X-ray Observatory (IXO)*. Such inner-shell processes, particularly K-shell processes, are observed in the spectral band of the observatories from all ionic stages of the most abundant elements. These spectra are extremely valuable for they can be used to diagnose the conditions of the plasma and its chemical composition. Until recently, however, atomic parameters for modeling K lines were not available. Over the last several years, our team has dedicated significant efforts toward the study of K-shell processes using different theoretical approaches, i.e. the relativistic Hartree-Fock (HFR) method, the AUTOSTRUCTURE code and the General Relativistic Atomic Structure Package (GRASP). Here we present an overview of our recent progress in ions of the N, Ne, Mg, Al, Si, S, Ar, Ca, Fe and Ni isonuclear sequences for which complete data sets of level energies, wavelengths, Einstein A-coefficients and Auger rates for K lines have been calculated. For some of these elements, K-shell photoionization cross sections were also computed using the Breit-Pauli R-matrix method.

2P060

Identification of electronic state of acetic acid in solution studied by X-ray emission spectroscopy

Y Horikawa,^{1,2} H Arai,¹ T Tokushima,¹ A Hiraya,² S Shin^{1,3}

¹RIKEN/SPring-8, Sayo-gun, Hyogo, Japan; ²Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan; ³ISSP, The University of Tokyo, Kashiwa, Chiba, Japan

The electronic structure is important for many fields of science because its determining role in materials property. Especially in chemistry and chemical physics, due to its importance, the number of studies on electronic structures in liquid using Photoemission (PES), X-ray absorption (XAS) and emission spectroscopy (XES) has been increasing recently. We have demonstrated site-specific observations of O(C=O) and O(OH) oxygen for liquid acetic acid under ambient conditions using XES through site-selective excitations [1]. This method was also applied to study acetic acid in aqueous solution. Occupied valence electronic structures in the neutral and the anionic forms of aqueous acetic acid and their pH dependence have been identified for the first time [2]. It was suggested from these two reports that electronic states of acetic acid molecule in solutions are not so much disturbed than expected. To investigate the solvation effect on the electronic states in detail, we observed the anisotropy of XES from acetic acid in solution using different polarization for excitation. Clear anisotropies of peak intensity were observed in resonant XES spectra. Symmetries of each peaks determined from measured anisotropy are consistent with the assignment of our previous reports [1,2]. Anisotropy ratio at an XES peak from HOMO fits quantitatively with the theoretical value expected for free molecules, and other peaks also show qualitative agreements.

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[2] Y. Horikawa *et al.*, *Phys. Chem. Chem. Phys.* 2009, **11**, 8676.

2P061

L-shell soft X-ray emission as incident X-ray photons are tuned across 1s ionization threshold

D Sokaras,¹ AG Kochur,² M Müller,³ M Kolbe,³ B Beckhoff,³ M Mantler,⁴ C Zarkadas,^{1,5} M Andrianis,¹ A Lagoyannis,¹ AG Karydas^{1,6}

¹Institute of Nuclear Physics, N.C.S.R. "Demokritos", Athens, Greece; ²Rostov State University of Transport Communication, Rostov-na-Donu, Russian Federation; ³Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany; ⁴Technische Universität Wien, Vienna, Austria; ⁵PANalytical B.V., Almelo, Netherlands; ⁶Nuclear Spectrometry and Applications Laboratory, International Atomic Energy Agency, Seibersdorf, Austria

The L-shell X-ray emission as an incident monochromatic radiation overpass the 1s ionization threshold is investigated for the metallic Fe by means of moderate resolution X-ray spectrometry. For the experimental study, polarized and unpolarized monochromatic X-ray beams provided by the PiXRF chamber at the Tandem accelerator laboratory of N.C.S.R. "Demokritos" as well as by the Four Crystal Monochromator beamline (PTB laboratory at BESSY II) were independently employed. A full ab initio theoretical investigation of the direct and the cascade L-shell X-ray emission spectrum was performed based on a detailed straightforward construction of the cascade decay trees within the Pauli-Fock approximation. The secondary ionizations induced by the ejected electrons to the neighboring Fe atoms were described through Monte Carlo calculations. For the self-attenuation corrections, experimental mass attenuation coefficients were obtained through transmittance measurements at the Plane Grating Monochromator beamline (PTB laboratory, BESSY II). The good agreement obtained between experiments and theory is indicated and discussed towards the characterization of modern technological nanomaterials through reference-free X-ray fluorescence analysis.

2P062

The change of Al $L_{2,3}$ at the welding interface between Al and Cu

S Fukushima,^{1,2} T Ogiwara,² H Shinotsuka,¹ T Kimura,¹ S Tanuma^{1,2}

¹ANCC, NIMS, Tukuba, Ibaraki, Japan; ²MAS, NIMS, Tukuba, Ibaraki, Japan

For the practical application of microanalysis with ultra-soft X-ray spectroscopy in the laboratory scale, this group has developed a general-purpose ultra-soft X-ray micro-analyzer with electron beam excitation, in the cooperation with JEOL Ltd. One of the recent applications using this apparatus is the observation of the welding interface between metallic Al and metallic Cu. From the result of the measurement with FE-WD-EPMA and the scatter diagram analysis, it was assumed that this interface was consisted of 3 phases of Al-Cu metallic compounds mainly; theta (Al_2Cu), eta (AlCu) and gamma ($AlCu_2$) phases. From the measurement of Al $L_{2,3}$, the relative signal intensity became weakened at the order of metal, theta, eta, gamma phase. The profile of metallic Al $L_{2,3}$ showed a good correspondence with the shape of total DOS calculated by WIEN 2k [band calculation], while that was not corresponding with the theoretical spectrum obtained by cluster (MO) calculation with DV-X α . The spectrum shapes obtained by subtraction of metallic Al spectrum from the spectrum of each phase showed good correspondence with each other and the result of the cluster calculation. The intensity of spectrum of metal for subtraction was the strongest in the case of theta phase, and weakened at the order of eta, gamma phases. From these results, we may conclude that the amount of conduction electrons in the vicinity of Al atom are decreased when the quantity of Cu is increased, and that the spectrum pattern of the alloy phases showed the shapes corresponding with the dipole transition from bonding orbitals directly.

2P063

Photoinduced $K\alpha$ hypersatellite X-ray emission for $12 \leq Z \leq 23$ elementsJ Hoszowska,¹ W Cao,¹ JC Dousse,¹ K Fennane,¹ Y Kayser,¹ M Kavčič,² J Szlachetko,³ M Szlachetko¹¹Physics Department, University of Fribourg, Fribourg, Switzerland; ²J. Stefan Institute, Ljubljana, Slovenia; ³European Synchrotron Radiation Facility, Grenoble, France

The radiative decay of double 1s vacancy states induced by single-photon impact was investigated for several low-Z elements (Mg, Al, Si, Cl, K, Ca, Sc and V). The $K\alpha$ hypersatellite X-rays ($1s^{-2}1s^{-1}2p^1$ transitions) were measured with the high-resolution Bragg-type bent crystal spectrometer of Fribourg [1] installed at the ID21, ID26 and BM05 beamlines at the European Synchrotron Radiation Facility (ESRF), Grenoble, France. The energies and natural linewidths of the $K\alpha^h$ hypersatellite lines were determined. A good agreement with the MCDF energies of Martins et al. [2] was observed, whereas the experimental widths were found to be underestimated by theory. The double-to-single photoionization cross section ratios as a function of the excitation energy were deduced from the relative hypersatellite intensities with respect to the parent diagram lines. A semiempirical universal scaling of the double photoionization cross sections was established [3].

[1] J. Hoszowska et al., Nucl. Instrum. Meth. Phys. Res. A 376 (1996) 129.

[2] M.C. Martins et al., J. Phys. B: At. Mol. Phys. 37 (2004) 3785.

[3] J. Hoszowska et al., Phys. Rev. Lett. 102 (2009) 073006.

2P064

Comparative study of soft X-ray photoabsorption, X-ray emission and UV-VUV luminescence in BeOA Kikas,¹ T Käämbre,¹ I Kuusik,¹ K Kooser,^{1,2} E Nõmmiste,¹ M Kirm,¹ E Feldbach,¹ V Kisand,¹ V Ivanov,³ V Pustovarov³¹Institute of Physics, University of Tartu, Tartu, Estonia; ²Department of Physics and Astronomy, University of Turku, Turku, Finland; ³Ural State Technical University-UPI, Ekaterinburg, Russian Federation

Insulating oxides have properties making them useful in a wide range of applications. BeO possesses high thermal stability, wide transparency and radiation resistance. It has also interesting electronic properties – several spatial configurations of self-trapped excitons and related luminescence bands have been identified. We present a comparative study soft X-ray photoabsorption, resonant X-ray emission and UV-VUV luminescence from BeO single crystals with incident photon energies in the vicinity of the Be 1s photoabsorption edge. The X-ray photoabsorption and emission measurements were carried out on beamline I511-3 at MAX-Lab, Lund (Sweden) and the luminescence experiments were performed at beamline BW3 in HASYLAB, DESY (Germany). Cathodoluminescence was studied using laboratory set-up in Tartu. The X-ray emission spectra show that at the Be 1s photoabsorption edge the lattice relaxation processes in the excitation site take place already on the time-scale of the radiative decay of the core excitation. Comparison of the X-ray emission and the luminescence spectra indicates that the maximum energy loss of the process of lattice relaxation during the decay of inner-shell holes is similar to the loss that occurs in the self-trapping process of valence excitons. The possible decay channels of core excitations have been discussed and the mechanism for the creation of 5.2 eV luminescence at the photoabsorption resonances has been suggested.

2P065

The features of the K-LM radiative Auger spectra of Cr, Fe, Co and Ni atomsNA Borovoy,¹ RM Ischenko¹¹Physical department, Shevchenko Kiev National University, Kiev, Ukraine

The K-LM radiative Auger effect (RAE) X-ray spectra of Cr, Fe, Co and Ni atoms are experimentally investigated by using of Bragg spectrometer with quartz curve-crystal. To separate the K-LM RAE satellites from the low-energy tail of $K\alpha_{1,2}$ lines the diagram $K\alpha_1$, $K\alpha_2$ lines and the $K\alpha_3$, $K\alpha_4$ satellites were approximated by four Voigt function. In the course of fitting, the width of the Gaussian component of the Voigt functions was maintained invariable and equal to the resolution of spectrometer, whereas all the remaining parameters were variable. It is found, that for atoms of these elements the structures of spectra are similar and are determined by two lengthy maxima: the high-energy maximum is more intensive, has a short-wave edge and is mainly caused by group of $K-L_{2,3}M_{1,2,3}$ radiative Auger-transitions; a group of the $K-L_1M_{1,2,3}$ radiative Auger-transitions causes the low-energy maximum. The relative intensities $\gamma = I(K-LM)/I(K\alpha_{1,2})$ of K-LM RAE satellites were determined as a ratio of the areas under the counters of K-LM satellites and $K\alpha_{1,2}$ lines. Relative probabilities of RAE, based on experimental γ values, are equal 0.43; 0.38; 0.34; 0.31 (%) for Cr, Fe, Co and Ni respectively that is 21-27 % below results of the calculations performed within the framework of sudden-perturbation approximation. Conclusion is made about necessity of the taking correlation effects into consideration at K-LM RAE description.

2P066

X-ray emission M_{α} and M_{β} spectra of Au, Pb and Bi atoms under electron impact near-threshold

NA Borovoy,¹ RM Ischenko¹

¹Physical department, Shevchenko Kiev National University, Kiev, Ukraine

The ratio of M_5N -satellites intensities to intensities of $M\alpha_{1,2}$ -lines along with the M_5O satellites (η_{α}), as well as the ratio of M_4N -satellites intensities to intensities of $M\beta$ lines along with the M_4O satellites (η_{β}) is experimentally investigated at electron bombardment of Au, Pb and Bi targets in energy range $E_0=5-30$ keV. The integral ionization cross sections (IICS) of Au, Pb and Bi M_i -subshells were calculated in plane-wave approximation (modified Bethe formula), classical momentum approximation (Gryzinski formula), according to the semiempirical Bethe formula [1] and used for calculations of η_{α} , η_{β} values of Au, Pb, Bi. It is found, that classical momentum approximation and semiempirical Bethe formula [1] with adjusting parameters for K- and L-shells are correct for calculation of M_i -subshells ionization cross sections at energies $E_0 > 10$ keV. However, in the near-threshold region $E_0=5-7$ keV significant distinctions between the experimental and calculated η_{α} , η_{β} values are observed. On the bases of experimental values η_{α} , η_{β} have been determined the most adequate values of adjusting parameters, which may be recommended for calculations of M -subshells IICS high elements $Z \geq 79$.

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2P067

Sensitivity of X-ray emission spectroscopy to hydrogen bonding: water in acetonitrile solvent

H Arai,^{1,2} Y Horikawa,² K Sadakane,³ Y Harada,^{2,4,5} T Tokushima,² Y Takata,^{1,2} S Shin^{2,6}

¹Department of Complexity Science and Engineering, University of Tokyo, Kashiwa, Chiba, Japan; ²RIKEN SPring-8 Center, Sayo-gun, Hyogo, Japan; ³Department of Physics, Kyoto University, Kyoto, Japan; ⁴Department of Applied Chemistry, University of Tokyo, Bunkyo-ku, Tokyo, Japan; ⁵JST, CREST, Kawaguchi, Saitama, Japan; ⁶ISSP, University of Tokyo, Kashiwa, Chiba, Japan

Recently, high resolution X-ray emission spectroscopy (XES) reveals that the spectrum of liquid water has two sharp peaks structure assignable to two types of hydrogen bonding configuration [1, 2]. The possible origin of two peaks is argued from the view point of initial and final state effect. In order to investigate the sensitivity of XES to hydrogen bonding, we studied electronic structure of liquid water in acetonitrile. While water molecule acts as proton donor and acceptor, acetonitrile acts only as proton acceptor. Hydrogen bonding of water is modified by the addition of acetonitrile. Thus, this system is suitable for investigating the sensitivity of XES to hydrogen bonding. All the experiments were performed at BL17SU in SPring-8. O 1s emission spectra change their shape by the addition of acetonitrile; the relative intensity of two peaks observed in liquid water gradually changes and the peak at higher energy position shows energy shift. This result shows the substitution of the bond from water-water to water-acetonitrile. At high acetonitrile concentration, two peaks are turned into one peak. This is consistent with IR study [3], i.e. water molecule exists as monomer. Water molecules are surrounded by acetonitrile molecules, and only donor hydrogen bonding is formed. These results confirmed the sensitivity of XES to hydrogen bonding.

[1] T. Tokushima et al., Chem. Phys. Lett. 460, 387-400 (2008). [2] C. Huang et al., PNAS 106, 15214 (2009). [3] D. Jamroz et al., J. Am. Chem. Soc. 115, 6165 (1993).

2P068

Charge transfer transitions in X-ray band emission of Mg compounds

RE Ovcharenko,¹ II Tupitsyn,¹ AS Shulakov¹

¹V.A.Fock Institute of Physics, Saint-Petersburg State University, Saint-Petersburg, Russian Federation

Calculations of Mg $L_{2,3}$ soft X-ray emission band spectra (SXES) have been performed for crystalline Mg, MgO, MgH₂, MgB₂ and MgF₂ by means plain wave method (code CASTEP) in the frame of LDA DFT using norm-conserving pseudopotentials. For matrix elements of X-ray transitions calculation procedure of so called all-electron orbitals reconstruction from pseudo-wave functions was utilized [1,2]. Calculations of radiative transition probabilities were fulfilled in two calibrations – in the length and velocity forms, what allowed to estimate errors bringing in by semi-local norm-conserving pseudopotentials and wave functions reconstruction procedure. Theoretical intensity distribution in Mg $L_{2,3}$ SXES are in a good agreement with experimental emission bands. Mg local partial density of states, s- and d- partial contributions to Mg $L_{2,3}$ SXES and partial Mg atomic occupancy were calculated as well. It was found what in Mg compounds d- contribution to Mg $L_{2,3}$ SXES significantly increases in relation to metallic Mg band. This increasing is proportional to the effective charge at ligand sites. We explain this phenomenon by presence (and contribution) of ligand ions electron states tails (mainly of p-symmetry) in the vicinity of Mg positive core ions. Therefore at least high photon energy part of Mg $L_{2,3}$ SXES in compounds may be regarded as charge transfer transitions.

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2P069

Electric-field induced insulator-metal transition in a Mott insulator Ca_2RuO_4 probed by resonant X-ray emission spectroscopy

N Nakajima,¹ M Sakaki,² F Nakamura,² Y Isohama,¹ H Maruyama,¹ Y Tezuka³

¹Grad. Sch. of Sci., Hiroshima Univ., Higashi-Hiroshima, Japan; ²ADSM, Hiroshima Univ., Higashi-Hiroshima, Japan; ³Grad. Sch. of Sci. & Tech. Hirosaki Univ., Hirosaki, Japan

Recently a quite unique dielectric breakdown nature has been reported in a 4d-electron Mott insulator Ca_2RuO_4 . The breakdown, insulator-metal transition, is induced by applying a small electric-field of $\mathcal{E}_{\text{th}} \sim 40$ V/cm and is accompanied by a first-order structural transition [1]. We can fully expect that these phenomena will make a great impact on not only basic physics but also application to electronic devices. There remain, however, many unsolved questions regarding the variation of the electronic states through the transition. In general, apical oxygen of the RuO_6 octahedron is expected to play an important role as is always the case with other perovskite oxides such as high- T_c cuprates, colossal magnetoresistive manganites and so on, hence the need for information about O 2p valence band. Resonant X-ray emission spectroscopy at the O K-edge was performed taking a full advantage of the photon-in photon-out technique which is free from any constraint of the applied field (\mathcal{E}). The conduction band as well as several core levels is observed by X-ray absorption spectroscopy (XAS) with the total and partial fluorescence yield modes. The \mathcal{E} -dependence measurements in the insulator phase were already done, where valence variation in Ca was evidenced from the peak splitting in XAS. Contrary to our expectation, both valence and conduction bands were not affected by \mathcal{E} . The measurements in the metallic phase are now in progress.

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2P070

A quantitative study of the Ni-L fluorescence processes by means of high-resolution soft X-ray emission spectrometry

M Müller,¹ B Beckhoff,¹ B Kanngießer²

¹Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany; ²Technical University of Berlin, Berlin, Germany

Well known atomic fundamental parameters (FP) such as fluorescence yields, transition probabilities, Coster-Kronig coefficients and partial photoelectric cross sections enable for a reliable quantitative description of fluorescence X-ray emission, e.g. with respect to advanced material characterizations. However, most of today's knowledge about these atomic FP is based on theory and experiments from 30 years ago. Especially in the soft X-ray range the reliability of the available data is debatable. Photon-in-photon-out investigations based on calibrated instrumentation can very well contribute to the traceable determination of such FP. This allows for the evaluation and improvement of theoretical calculations, e.g. the L fluorescence processes of transition metals are strongly affected by solid state effects while the available theory for the calculation of these FP is mostly valid for free atoms only. The determination of the full set of atomic FP associated with the L-fluorescence X-ray emission of Ni was performed employing an absolutely calibrated high-resolution wavelength-dispersive spectrometer [1]. Taking advantage of the tunability of monochromatized undulator radiation, a quantitative study of the evolution of the Ni-L emission spectrum with increasing incident photon energy in the range of the L absorption edges was conducted. In particular, the $L\alpha$ satellite emission could be quantified separately in respect to the originating Coster-Kronig and shake processes.

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2P071

Electronic properties of $\text{FeSe}_{1-x}\text{Te}_x$ single crystals

CL Dong,¹ CL Chen,² JL Chen,³ TW Huang,² KW Yeh,² WL Yang,³ JH Guo,³ SM Rao,² MK Wu²

¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Institute of Physics, Academia Sinica, Taipei, Taiwan;

³Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

In the young and rapidly developing field of new discovered Fe-based superconductor, an important issue that needs to be understood is whether the Fe-based superconductors are strongly correlated system like the cuprates. We have used the X-ray absorption (XAS) and resonant inelastic X-ray scattering (RIXS) to investigate the electronic properties of $\text{FeSe}_{1-x}\text{Te}_x$ ($x=0\sim 1$) single crystals. The XAS has been demonstrated to be a powerful tool for probing the crystal field and electronic interaction for 3d transition metals. In addition, the excitation-induced energy loss features in the RIXS spectrum can be viewed as an indicator of the strength of electron correlation. For a direct comparison of the XAS and RIXS spectra of Fe metal, Fe_2O_3 and $\text{FeSe}_{1-x}\text{Te}_x$ single crystals, it suggests the Fe-based superconductors are unlikely to be strongly correlated systems.

2P072

The valence band electronic structure of RuO₂ - A study of chemical bonding through polarisation dependent resonant soft X-ray emission

C McGuinness,¹ B Kennedy,¹ D Cockburn,¹ B Arnold,¹ JD Denlinger,² T Käåmbre,^{3,4} R Egdell⁵

¹School of Physics, Trinity College Dublin, Ireland; ²Advanced Light Source, Lawrence Berkeley Laboratory, United States; ³MAX-lab, Lund University, Sweden; ⁴Institute of Physics, Tartu University, Estonia; ⁵Department of Chemistry, Oxford University, Great Britain

RuO₂ is a metallic oxide that forms in a rutile-type crystal structure with octahedral coordination of the metal cations (RuO₆) and a trigonal planar coordination of the oxygen anions (Ru₃O). As a result of this trigonal planar coordination the oxygen anions become sp² hybridised giving rise to σ-like metal-oxygen molecular orbitals in the Ru3O plane, and π-like metal-oxygen orbitals perpendicular to this plane. As these planes all contain the c-axis, there is a natural linear dichroism at the oxygen K-edge which can be observed in X-ray absorption (XAS) from an oriented single crystal. This natural linear dichroism is analogous to that already reported for CrO₂ as both materials have O 2p orbitals hybridised with a partially occupied metal t_{2g} band, respectively for CrO₂ and RuO₂ due to a 3d² Cr ion and a half-metallic band structure, a 4d⁴ Ru ion with a fully metallic band structure. Reported here is a detailed spectroscopic study of the bulk electronic structure of RuO₂ obtained by oxygen K-edge XAS, and by the combination of this with polarisation dependent resonant soft X-ray emission spectroscopy (RXES) also at the oxygen K-edge. These measurements have been obtained both in an in-plane and out-of plane scattering geometries and the results compared to O 2p partial densities of states obtained from density functional theory calculations. Appropriate linear combinations of the observed RXES spectra measure the individual O 2p densities of states projected along three orthogonal axes: along the Ru-O axis to the apical O; along the c-axis (both within the Ru₃O plane); and perpendicular to the Ru₃O plane. The observed RXES is polarisation dependent, symmetry selective, but also exhibits k-selectivity due to bandstructure providing insight into the chemical bonding within the bulk electronic structure of RuO₂.

2P073

Concept of spectrometer for soft-X-ray RIXS with parallel detection in incoming and outgoing photon energies

VN Strocov¹

¹Swiss Light Source, Paul Scherrer Institute, Switzerland

A concept of spectrometer for resonant inelastic X-ray scattering (RIXS) in the soft-X-ray range is proposed where imaging and dispersion actions in two orthogonal planes are combined to deliver in one shot the full two-dimensional map of RIXS intensity as a function of incoming $h\nu_{in}$ and outgoing $h\nu_{out}$ photon energies. Optical scheme of such a next generation RIXS instrument – nicknamed $h\nu^2$ -spectrometer – uses plane-elliptical KB optics in the refocusing stage and a plane-elliptical focusing mirror combined with spherical VLS grating in the spectrometer stage. Preliminary ray-tracing simulations with a typical 3rd generation synchrotron source demonstrate a resolving power well above 11000 in both $h\nu_{in}$ and $h\nu_{out}$ near 930 eV, with a vast potential for improvement with better horizontal refocusing. Furthermore, the detection channel in $h\nu_{out}$ can be utilized as a means to increase the detection efficiency by a factor ~50 compared to the conventional instruments. By virtue of the one-shot operational principle of the $h\nu^2$ -spectrometer, its installation at XFEL sources allows efficient time-resolved RIXS experiments. The low emittance and round spot profile of these sources simplify technical implementation of the spectrometer.

V.N. Strocov, J. Synchrotron Rad. **17** (2010) 103

2P076

Influence of the X-ray energy on the shape of the d-metal valence bands

I Shabanova¹

¹Physicotechnical Institute, Ural Division of Russian Academy of Sciences, Izhevsk, Russian Federation

The photoionization cross-section of the valence electrons with different symmetry depends on the energy of exciting radiation. In order to find the parameters of the X-ray photoelectron spectra, which are sensitive to the change of chemical bond, the study of the influence of the X-ray radiation energy on the shape of the X-ray photoelectron spectra of valence bands has been conducted for a number of d-metals. Using Cu, Ni, Fe and Ti as examples, the dependence of the shape of the valence band spectra on the radiation energy exciting photoelectrons is shown. This dependence is associated with the predominant probability of the photoionization of d-electrons with the symmetry e_g and t_{2g}. The e_g-electron contribution significantly increases with an increase in the energy of radiation (from 40.8 eV to 4510 eV). It is known that e_g-electrons participate in the formation of the directed covalence s bond Me-X at the overlapping of e_g and p_s orbitals. The metal-type bonds are realized by t_{2g}-electrons. Therefore, for the investigation of the interatomic bond of 3d atoms with the environment by valence band spectra, it is necessary to use high-energy radiation (hard radiation) for exciting electrons.

2P077

Exploring the Fe-MgO interface using photoemission with X-ray standing-wave excitation

S Döring,¹ F Schönbohm,¹ U Berges,¹ D E Bürgler,² C M Schneider,² M Gorgoi,³ F Schäfers,³ W Braun,³ CS Fadley,⁴ C Westphal¹

¹Exp. Physik 1 and DELTA, TU Dortmund, Dortmund, Germany; ²Institut für Festkörperforschung IFF-9 and JARA-FIT, Forschungszentrum Jülich, Jülich, Germany; ³Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ⁴LBNL, Berkeley, CA, United States

We present recent results of our studies on the Fe-MgO interface. This interface is of central importance for *magnetic tunnel junctions* (MTJs). For a better understanding of the *tunnel-magneto-resistance* (TMR) effect it is essential to identify the chemical states of Fe, Mg, and O atoms at the interface. Especially the formation or non-existence of FeO is a crucial parameter for theoretical models of the TMR effect in MTJs. Investigating the chemical states of atoms at buried interfaces is still a major challenge in today's research. The combination of photoemission with the X-ray standing-wave technique improves the depth-resolution and opens the door to truly interface sensitive studies. In the present study we deposit a wedge-shaped Fe-layer and cover it by a MgO-film. Thus, when the sample is moved perpendicular to the beam direction, the Fe-MgO interface of interest is lifted through the standing-wave field and experiences high and low light intensity at different lateral positions. We report for the first time an investigation of the chemical states of atoms at the buried Fe-MgO interface by a combined photoemission and standing-wave study. From the quantitative analysis of our data we find a rather narrow intermixing region and no indication for the Fe-oxidation at the interface.

2P078

Electronic structure and magnetic property of Fe-doped ZnO film grown by laser-MBE

T Chen,¹ F Xu,¹ L Cao,¹ W Zhang,¹ Y Han,¹ Z Zheng,¹ K Ibrahim,² J Wang²

¹National Synchrotron Radiation Laboratory, USTC, Hefei, Anhui, China; ²Synchrotron Radiation Laboratory, Institute of High Energy Physics, the Chinese Academy of Sciences, Beijing, China

Fe-doped ZnO film is grown by laser-MBE and structural characterized by X-ray diffraction and scanning electron microscopy. Resonant photoelectron emission spectroscopy (RPES) with photon energy from 698eV to 730eV is detected at the region of ZnO valence band to unravel the Fe 3d states in the valence band. It is argued that the spectrum shows a strong resonant effect with respect to the absorption from Fe2p to Fe3d states at the photon energy of 710eV. The Fe3d states are detected from the spectrum. Magnetization measurements of M-H curve on the system are performed and it shows a superparamagnetism property. Theory analysis has been done to elaborate on the origin of the magnetic property linking to the photoelectron emission spectroscopy.

2P079

High energy photoemission spectroscopy facility at SXRMB beamline of CLS

QF Xiao,¹ YB Shi,^{1,2} YF Hu,¹ TK Sham³

¹Canadian Light Source, Saskatoon, SK, Canada; ²Institute of Physics, Chinese Academy of Sciences, Beijing, China; ³Department of Chemistry, The University of Western Ontario, London, Ontario, Canada

Canadian Light Source is developing the high energy X-ray photoemission spectroscopy (HXPES) facility at Soft X-ray Micro-characterization Beamline (SXRMB). The SXRMB uses a bending magnet source, and with InSb(111) and Si(111) crystal monochromator to cover the energy range of 1.7 – 10.0 KeV. It is designed to have a resolving power of 10^4 , a flux of 10^{12} photons/500mA/Sec and a spot size of $< 1 \times 1 \text{ mm}^2$ at the sample. The beamline is optically commissioned and is open to general users for X-ray photoabsorption experiments. The HXPES system is being designed and built and it will consist of the following major components: (a) a VG SCIENTA R4000 electron analyser that is used for electron kinetic energies from a few eV up to 10 keV; (b) a UHV main chamber with the analyzer mounted 90 degrees to the incident beam; (c) a VG SCIENTA Cryoax 5 manipulator with 5 movements (x, y, z, primary rotation and azimuthal rotation); and (d) a motorized chamber support with four movements (x, z, roll and pitch). This HXPES system is expected to be in commission in spring of 2011.

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2P080

Breakdown of the dipole approximation and determination of individual sub-shell cross-section for hard X-rays

J Rubio-Zuazo,^{1,2} GR Castro^{1,2}

¹CRG SpLine at the ESRF, Grenoble, France; ²Instituto de Ciencia de Materiales de Madrid-CSIC, Madrid, Spain

Hard X-ray Photoelectron Spectroscopy (HAXPES) is a powerful emerging technique for bulk compositional, chemical and electronic properties determination. It benefits from the exceptionally large escape depth of high kinetic energy photoelectrons enabling the study of bulk and buried interfaces up to several tens of nanometers depth. HAXPES also gives the opportunity to analyze the photoionization process from a different point of view than when using soft X-rays. For Hard X-rays several parameters play an important role on the photoionization process such as the evaluation of the breakdown of the dipole approximation or the absolute determination of the individual sub-shells cross-section. In this work we present an evaluation of the breakdown of the dipole approximation involved on the photoemission process. For that we have measured the angular distribution of the emitted photoelectrons within a photon energy range from 7–26 keV and photoelectron kinetic energy range 1–15 keV. In the case of Gold, a shift to the forward direction (photon direction) of the photoelectron angular distribution maximum is present which cannot be explained by the dipole approximation. Secondly, we will present a systematic study of the individual subshell photoionization cross-sections as a function of the involved atomic level, atomic number, photon energy, element and photoelectron kinetic energy within the mentioned photon energy and photoelectron kinetic energy range. For the case of Gold, the cross-section dependency with the photon energy deviates from the Bethe theory for photon energies above 7 keV.

2P081

Interface-sensitive X-ray spectroscopy of oxide heterostructures: HAXPES and RIXS applied to LaAlO₃/SrTiO₃

R Claessen¹

¹Physikalisches Institut, Universität Würzburg, Würzburg, Germany

Oxide heterostructures combine the electronic and magnetic properties of transition metal oxides with the opportunities of atomic precision heteroepitaxy by pulsed laser deposition (PLD). By suitable choice of materials it is possible to generate two-dimensional electron systems (2DES) at the heterostructure interface with tunable properties. A case in point is the system LaAlO₃/SrTiO₃ (LAO/STO), where between two insulators a high-mobility 2DES forms, whose carrier density can be controlled by field effect and which displays switchable superconductivity at low temperatures. Spectroscopic investigations of such 2DES require suitable methods with sufficient interface sensitivity. Here I will demonstrate that synchrotron-based hard X-ray photoelectron spectroscopy (HAXPES) and resonant inelastic X-ray scattering (RIXS) are highly valuable tools for this purpose. As an example I will discuss the application of HAXPES and RIXS to the LAO/STO system [1,2], yielding important information on orbital nature, carrier density, and spatial extent of the 2DES.

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2P082

Hard-x-ray photoelectron spectroscopy study on role of electronic structure in the martensitic phase transition of Ni₂Mn_{1+x}Sn_{1-x}

M Ye,¹ A Kimura,¹ Y Miura,² M Shirai,² YT Cui,³ K Shimada,³ H Namatame,³ M Taniguchi,^{1,3} S Ueda,⁴ K Kobayashi,⁴ R Kainuma,⁵ T Shishido,⁶ K Fukushima,⁷ T Kanomata⁷

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Research Institute of Electrical Communication, Tohoku University, Sendai, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ⁴NIMS Beamline Station at SPring-8, National Institute for Materials Science, Sayo, Hyogo, Japan; ⁵Institute for Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan; ⁶Institute for Materials Research, Tohoku University, Sendai, Japan; ⁷Faculty of Engineering, Tohoku Gakuin University, Tagajo, Miyagi, Japan

We have revealed the underlying mechanism of the martensitic phase transition (MPT) in a new class of ferromagnetic shape memory alloys, Ni₂Mn_{1+x}Sn_{1-x}, by the combination of bulk-sensitive hard-x-ray photoelectron spectroscopy and a first-principles density-functional calculation. The Ni 3d e_g state in the cubic phase systematically shifts towards the Fermi energy with an increase in the number of Mn atoms substituted in the Sn sites. An abrupt decrease of the intensity of the Ni 3d e_g states upon MPT for x = 0.36–0.42 has been observed in the vicinity of the Fermi level. The energy shift of the Ni 3d minority-spin e_g state in the cubic phase originates from hybridization with the antiferromagnetically coupled Mn in the Sn site. Below the MPT temperature, the Ni 3d state splits into two levels located below and above the Fermi energy in order to achieve an energetically stable state.

2P083

Evidence for the constancy of U in the Mott transition of V_2O_3 revealed by hard X-ray photoemission

H Fujiwara,^{1,2} A Sekiyama,^{1,3} SK Mo,^{4,5} JW Allen,⁴ J Yamaguchi,¹ G Funabashi,¹ S Imada,¹ P Metcalf,⁶ A Higashiya,³ M Yabashi,^{3,7} K Tamasaku,³ T Ishikawa,³ S Suga^{1,3}

¹Graduate School of Engineering Science, Toyonaka, Osaka, Japan; ²Il. Physikalisches Institut, Universitaet zu Koeln, Koeln, Germany; ³SPring-8/RIKEN, Sayo, Hyogo, Japan;

⁴Randall Laboratory of Physics, University of Michigan, Ann Arbor, Michigan, United States; ⁵Department of Physics, Stanford University, Stanford, California, United States;

⁶Department of Physics, Purdue University, West Lafayette, Indiana, United States; ⁷SPring-8/JASRI, Sayo, Hyogo, Japan

V_2O_3 is a paradigmatic example of Mott-Hubbard metal-insulator transition [MH-MIT] materials with a very rich phase diagram as a function of temperature, pressure and Ti- or Cr-doping. Nevertheless, the underlying physics is not trivial because of the strong interplay among charge-, spin- and orbital-degrees of freedom. We have carried out high-resolution hard X-ray photoemission spectroscopy (HAXPES) for $(V_{1-x}Cr_x)_2O_3$ ($x=0, 0.015$) in the paramagnetic metal, paramagnetic insulator and antiferromagnetic insulator phases. The measurements were performed at BL19LXU in SPring-8 with total energy resolution of 130 meV. Spectral weight transfers for the bulk V 3d states are observed across all phase boundaries, enabling identification of the lower Hubbard band in the spectra for all three phases. Thereby we have revealed that the on-site Coulomb energy U does not change through the metal-insulator transitions. This finding adds validity to the idea of the orbital selective Mott-transition in $(V_{1-x}Cr_x)_2O_3$.

2P084

Bulk sensitive photoemission and core-level magnetic dichroism of iron

S Imada,¹ K Terashima,¹ R Yamaguchi,¹ Y Miyata,¹ K Mima,¹ R Machino,¹ A Higashiya,² A Yamasaki,³ Y Matsui,³ A Sekiyama,⁴ J Yamaguchi,⁴ H Sugiyama,⁴ S Suga,⁴ M Yabashi,^{5,6} K Tamasaku,⁵ T Ishikawa,⁵ T Watanabe,⁷ K Mibu⁸

¹Ritsumeikan University, Kusatsu, Shiga, Japan; ²WINTEC, Wakayama, Wakayama, Japan; ³Konan University, Kobe, Hyogo, Japan;

⁴Osaka University, Toyonaka, Osaka, Japan; ⁵RIKEN, Sayo, Hyogo, Japan; ⁶JASRI, Sayo, Hyogo, Japan; ⁷Nihon University, Chiyoda-ku,

Tokyo, Japan; ⁸Nagoya Institute of Technology, Nagoya, Aichi, Japan

Iron compounds are attracting much more attention since the discovery of iron pnictide superconductors. Photoemission has long been a powerful tool for elucidating the iron 3d electronic states in such compounds. Especially, access to the genuine bulk properties has been opened by the recent development of hard X-ray photoemission. We have carried out hard X-ray photoemission of pure iron and iron compounds with use of photons of about 8 keV. The lineshape of Fe 2p XPS is compared between systems in which iron is magnetic and nonmagnetic. Magnetic circular dichroism in Fe 2p XPS of pure iron has further been studied. Linear polarization dependence of valence photoelectron spectrum of pure iron has also been studied. As a magnetic (nonmagnetic) iron system, pure iron ($Lu_2Fe_3Si_5$) has been chosen. With the total resolution of about 0.2 eV, the width of the Fe 2p_{3/2} XPS peak of $Lu_2Fe_3Si_5$ was only about 0.6 eV. On the other hand, that of pure iron was as large as about 1.4 eV, with a clear shoulder at about 0.9 eV higher binding energy from the peak. In order to check that the origin of the 0.9-eV shoulder is magnetism, we have measured magnetic circular dichroism (MCD) of Fe 2p XPS. A prominent MCD effect is observed; the relative intensity ratio between the main peak and the shoulder structure depends drastically on the magnetization direction. This clearly shows that the origin of the shoulder structure is the Fe 3d magnetic moment. Finally, the Fe 4s and 3d contributions to the valence band photoelectron spectrum are shown to be evaluated by measuring linear polarization dependence.

2P085

Anisotropic occupation of orbitals in $CeRh_3B_2$ studied by polarization-dependent photoemission

K Mima,¹ Y Miyata,¹ R Yamaguchi,¹ A Yamasaki,² A Sekiyama,³ S Suga,³ A Higashiya,⁴ T Muro,⁵ K Terashima,¹ M Yabashi,^{6,5} K Tamasaku,⁶ T Ishikawa,⁵ M Sakoda,⁷ E Matsuoka,⁷ H Sugawara,⁷ S Imada¹

¹Ritsumeikan University, Kusatsu, Shiga, Japan; ²Konan University, Kobe, Hyogo, Japan; ³Osaka University, Toyonaka, Osaka, Japan; ⁴WINTeC, Wakayama, Wakayama, Japan;

⁵JASRI/SPring-8, Sayo, Hyogo, Japan; ⁶RIKEN, Sayo, Hyogo, Japan; ⁷Kobe University, Kobe, Hyogo, Japan

$CeRh_3B_2$ exhibits a ferromagnetic transition at an exceptionally high Curie temperature ($T_c = 115$ K) among the Ce compounds with no transition metal magnetic element [1]. The magnetization measurement shows that the sample holds a magnetic moment of $0.56 \mu_B/f.u.$ at 4.2 K, whose direction is perpendicular to the *c*-axis [2]. It is argued from the self-consistent band calculation result that the main origin of the magnetic moment is not the Rh 4d electrons, but the Ce 4f electrons [3]. The calculation also predicts that the Ce 4f orbital pointing to the *c*-axis is preferentially occupied. In order to evaluate the anisotropy in the valence band electronic states, we have performed a photoemission study on $CeRh_3B_2$ using linearly polarized soft and hard X-rays respectively at BL27SU and BL19LXU of SPring-8. Strong polarization dependence was found in both soft and hard X-ray photoemission, which gives, according to the selection rule, a direct evidence of the anisotropic occupation of Ce 4f and Rh 4d bands. The polarization dependence shows that *m*=0 orbital [pointing to the *c*-axis] is preferentially occupied among the Ce 4f orbitals. We have also carried out bulk-sensitive Ce 3d XPS using hard X-ray, from which the weights of Ce 4f⁰, 4f¹ and 4f² states are directly estimated.

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2P086

Hard X-ray photoelectron spectroscopy as a nondestructive in-depth method for the buried interfaces study

E Filatova,¹ A Sokolov,¹ M Gorgoi,² F Schaefer²

¹V.A.Fock Institute of Physics, St. Petersburg State University, St. Petersburg, Russian Federation;

²Helmholtz Zentrum Berlin für Materialien und Energie (HZB-BESSY II), Berlin, Germany

X-ray photoelectron spectroscopy is a technique in common use for surface analyze. A key question in any photoemission experiment is the sample depth sensitivity that traditionally is related to the photoelectron inelastic mean free path, which is defined as the average distance that an electron with a given kinetic energy travels between successive inelastic collisions. With increasing kinetic energy, the mean free path of the electrons increases significantly that opens the possibility for investigation of deeply buried interfaces in samples. There is a question what the information (maximum) depth, normal to the surface, from which useful information can be obtained? It was established that depth sensitivity can be essentially varied by changing the photoelectron's emission angle and kinetic energy. It will be demonstrated that High Kinetic Energy - Hard X-ray Photoelectron Spectroscopy (HIKE or HAXPES) is a very effective non-destructive in-depth technique for chemical analysis of layered systems which allows detecting the presence of deeply buried interfaces. The possibility of estimation of the individual thicknesses of all the layers involved on the basis of the peak areas of different core levels will be discussed. The results for TiO₂/SiO₂/Si, Ti/SiO₂/Si and HfO₂/Si samples will be discussed. This work was supported by the ISTC (Project No 3963).

2P087

Bias-voltage application in hard X-ray photoelectron spectroscopy for characterization of advanced materials

Y Yamashita,^{1,2} H Yoshikawa,¹ S Ueda,¹ T Chikyow,² K Kobayashi¹

¹NIMS Beamline Station at SPring-8, National Institute for Material Science, Sayo, Japan;

²Advanced Electronic Materials Center, National Institute for Material Science, Tsukuba, Japan

We employed bias-voltage-application in hard X-ray photoelectron spectroscopy (BA-HXPES) to detect electronic states of materials in operating devices. To demonstrate the versatility of this method, we used a metal/SiO₂/Si(100) structure as a prototype and found that electronic states at the SiO₂/Si(100) interface were changed depending on the bias-application to the structure. By analyzing the change as a function of bias-voltage, the interface electronic states in the whole Si gap have been directly obtained in which these states can not be detected without the bias-application. Additionally we successfully obtained local potential distribution in high-k based gate-stack structures by means of this method. Therefore this approach could be applicable to various kinds of advanced materials and will be indispensable for evaluating their properties in detail. BA-HXPES is a new method to characterize electronic states for advanced materials under device operation.

2P089

X-dependent electronic structure of YbXCu₄ (X=Cd, In, Sn) investigated by hard X-ray photoemission spectroscopy

Y Utsumi,¹ H Sato,² K Tobimatsu,¹ H Maso,¹ K Hiraoka,³ K Kojima,⁴ K Mimura,⁵ S Ueda,⁶ Y Yamashita,⁶ H Yoshikawa,⁶ K Kobayashi,⁶ K Shimada,² H Namatame,² M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³Graduate School of Science and Engineering, Ehime University, Matsuyama, Japan; ⁴Graduate School of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima, Japan; ⁵Graduate School of Engineering, Osaka Prefecture University, Sakai, Japan; ⁶NIMS Beamline Station at SPring-8, National Institute for Materials Science, Hyogo, Japan

YbInCu₄ exhibits valence transition at $T_v \sim 42$ K, where the mean valence of Yb changes from $z \sim 3$ in high temperature (HT) phase to $z \sim 2.9$ in low temperature (LT) phase. Recently, we have performed hard X-ray photoemission (HX-PES) taken at $h\nu \sim 6$ keV for YbInCu₄, and found the Cu 2p and In 3d spectra shift toward E_F by 40 and 30 meV in LT phase, respectively, suggesting that conduction electrons at the Cu and In sites move to the Yb 4f orbitals at T_v [1]. In this study, we have investigated the electronic structures of YbCdCu₄ and YbSnCu₄ with no valence transition by HX-PES at BL15XU of SPring-8, and compared them with that of YbInCu₄. The Yb mean valences of YbCdCu₄ and YbSnCu₄ at 300 K derived from the Yb 3d spectra are close to HT and LT phases of YbInCu₄ (2.95 and 2.85), respectively, and continuously decreases on cooling. Regarding the Cu 2p spectra, we found that they shift away from E_F with increasing 5p electron (from Cd to In and to Sn), indicating the increased electron partly distributes over the Cu sites. As the 3d core levels for Yb²⁺ are almost unchanged for these materials, it is considered that the Cu conduction electrons play an important role for the valence transition of YbInCu₄, compared with the Yb conduction electrons.

[1] Y. Utsumi *et al.*, in preparation.

2P090

Hard X-ray photoelectron spectroscopy, first principle calculation, and chemical bonding in phase change memory materials $(\text{GeTe})_{1-x}(\text{Sb}_2\text{Te}_3)_x$

K Kobayashi,¹ JJ Kim,² J Akola,³ R O Jones,⁴ E Ikenaga,² M Kobata,¹ S Ueda,¹ S Kohara,² T Matsunaga,⁵ R Kojima,⁵ N Yamada⁵

¹National Institute for Materials Science, Sayo, Hyogo, Japan; ²Japan Synchrotron Radiation Research Institute/SPring-8, Sayo, Hyogo, Japan; ³Nanoscience Center, Department of Physics, University of Jyväskylä, Mattilanniemi, Finland; ⁴Institut für Festkörperforschung, Forschungszentrum, Jülich, Germany; ⁵Panasonic Corporation, Moriguchi-shi, Osaka, Japan

Fast and reversible phase change (PC) in $(\text{GeTe})_{1-x}(\text{Sb}_2\text{Te}_3)_x$ (GST) pseudo-alloys makes them very ubiquitous in rewritable optical storage devices such as DVD and Blue-ray disc. Large scale integrated devices are also under development in advanced semiconductor industries. However, the mechanism of the NaCl cubic (C) to amorphous (A) phase change has not yet been well understood. Umbrella flip model, in which change of the octahedral bonding of Ge in C-phase into sp^3 like tetrahedral configurations supposed to take place randomly at quenching, has been proposed by Kolobov et al. [1] based upon XAFS analysis. Hard X-ray photoelectron spectroscopy (HXPS) of the GST alloys [3] has revealed that valence band spectra of C- and A-phases resemble each other, exhibiting a broad p -like band and well separated lone pair s -band. This result makes a clear contrast to the Si case where difference in spectral shapes is obvious between C- and A-phases. Very recently, we have performed large scale DFT calculations, applying atomic structural constriction based upon RMC analysis of XRD result in A-phase. Here we present comparison of the HXPS and DFT results, discussions on the electronic structures of C- and A-phases and the phase change mechanism, in relation with a specific chemical bonding in the average 5 valence electron materials.

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2P091

Development of laboratory hard X-ray photoelectron spectroscopy system and application to measurement of SiO_2 thickness on Si(001)

M Kobata,¹ I Piš,^{1,2} H Iwai,³ H Yamazui,⁴ H Takahashi,⁴ M Suzuki,⁴ H Hohira,⁵ H Matsuda,⁶ H Daimon,⁶ K Kobayashi¹

¹National Institute for Materials Science, SPring-8, BL15XU, Sayo, Hyogo, Japan; ²Charles University, Prague, Czech Republic; ³National Institute for Materials Science, Tsukuba, Ibaraki, Japan; ⁴ULVAC-PHI, INC., Chigasaki, Kanagawa, Japan; ⁵Tokyo City University, Setagaya-ku, Tokyo, Japan; ⁶Nara Institute of Science and Technology, Ikoma, Nara, Japan

We report development of a practical laboratory hard X-ray photoelectron spectroscopy (HXPS) system by combining a focused monochromatic Cr K α X-ray source, a wide angle acceptance objective lens [1] and a high kinetic energy electron analyzer. The total resolution of 0.53 eV was estimated by Au Fermi-edge measurements. Angle acceptance of $\pm 35^\circ$ with an angular resolution of 0.5° was verified. The Si 1s photoelectrons from a Si(001) substrate at a kinetic energy of 3569 eV was clearly observed even through a 20-nm-thick overlayer, showing the possibilities of deeper (larger) detection depth with the designed system. Take-off angle (TOA) dependences of Si 1s spectra of $\text{SiO}_2/\text{Si}(001)$ samples in angular resolution mode were measured in the TOA range of $0-70^\circ$. The relative intensity of the oxidized states of Si 1s spectra to that of substrate Si 1s spectra were changed in accordance with the TOA. Thickness values of the SiO_2 overlayers determined by the method described above coincide excellently with those determined by ellipsometry. The acquisition time was *ca.* 60 min, with sufficient S/N for the determination of SiO_2 overlayer thickness. The HXPS system was proved to be a promising tool for the analysis of oxide layer thickness in the region of 1-20 nm. Moreover, this system is expected to have wide applicability for the investigation of electronic structure and chemical states of bulk and thin solid film materials. This work is supported by SENTAN, JST.

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2P092

Hard X-ray high kinetic energy photoelectron spectroscopy in BESSY II - recent results

M Gorgoi,¹ F Schaefer,¹ A Föhlisch¹

¹BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Recently, hard X-ray high kinetic energy photoelectron spectroscopy has led to a break-through in the field of photoemission due to its non-destructive way of investigating the bulk electronic properties of materials and in particular buried interfaces. In the present contribution we will report recent experiments performed at the hard X-ray High Kinetic Energy (HIKE) photoelectron spectroscopy facility at the Berliner synchrotron light source BESSY II. The facility successfully combines the bending magnet source of the KMC-1 beamline with a new generation electron spectrometer optimized for high kinetic energy electrons. Several topics will be detailed such as the sub-shell photoionization cross sections of selected metals at high energies and the recoil effect of high energy photoelectrons from light elements as a function of excitation energy within the range of 2 to 9 keV as well as other examples from material science.

2P093

Vibrational structure of the C 1s⁻¹ photoelectron line of CO

YS Krivosenko,¹ AA Pavlychev¹¹Department of Physics, St. Petersburg State University, St. Petersburg, Russian Federation

The influence of the shakeup C 2σ⁻¹1π⁻¹2π¹ (²Σ⁺) states on spectral distribution of vibrational excitations associated with C 1s ionization in the CO molecule is studied. A new mechanism of non-Franck-Condon distributions originated from the coupling of the core-ionized-valence-excited states via autoionization to C 1s⁻¹ continuum is revealed. This mechanism is expected to be general. The work of the mechanism is considered and it is shown that the Franck-Condon principle is not longer applicable to the transitions to v⁺≥4 vibrational states. As a consequence of the valence shells relaxation, striking changes are predicted in the vibrational structure of the C 1s photoelectron line relative to the Franck-Condon distribution of vibrational transitions in CO. The performed calculations demonstrate appearance of a non-Franck-Condonian shoulder from the low kinetic energy side of the vibrational envelop of the C 1s photoelectron line. Comparison with experimental spectra is discussed. High energy X-ray photoelectron spectroscopic studies of the low intense transitions are regarded as the most promising tool to reveal the extended shoulder and to check the work of the non-Franck-Condon mechanism.

2P094

Photoelectron diffraction patterns from ZnO and Si single crystals at high kinetic energies

I Pis,^{1,2} M Kobata,² T Matsushita,³ J Williams,⁴ E Ikenaga,³ T Sugiyama,³ K Kobayashi²

¹Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic; ²Beamline Station at SPring-8, National Institute for Materials Science, Sayo, Hyogo, Japan; ³Japan Synchrotron Radiation Research Institute, SPring-8, Sayo, Hyogo, Japan; ⁴International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Ibaraki, Japan

Photoelectron diffraction at high energies extends the applicability of this local atomic structure sensitive technique to new materials. The drawback of a low photoelectron intensity in the hard X-ray regime has been overcome by using high-brilliance synchrotron radiation sources. In addition, the recently developed laboratory system with Cr Kα X-source [5.4 keV] [1] is verified to provide a practical throughput for the hard X-ray photoelectron spectroscopy. We present polar-azimuth photoelectron diffraction patterns detected at an electron kinetic energy range of about 3.6~7.4 keV from Si(001), wurtzite-type ZnO(0001), and ZnO(000-1) single crystals. The large escape depths of the photoelectrons at such kinetic energies provide us bulk-sensitive measurements. The measurements were done at undulator beamline BL47XU of SPring-8. We also report results obtained by the Cr Kα X-source laboratory system [2]. The measured data will be compared with simulations based on a cluster model calculation. This work was supported by "Charles University-NIMS Joint Graduate School Program" and "SENTAN" JST. The authors are grateful to M. Machida, J. Y. Son, Y. Watanabe of JASRI, H. Matsuda, H. Daimon of NAIST, and H. Nohira of TCU for their cooperation. [1] M. Kobata *et al.*: Anal. Sci.26 [2010] 227. [2] I. Pis *et al.*: Appl. Phys. Express, to be published.

2P095

Bulk electronic structure of (Ga,Mn)As ferromagnetic semiconductors via angle-resolved hard X-ray photoemission

PR Stone,^{1,2} AX Gray,^{1,3} S Ueda,⁴ Y Yamashita,⁴ J Fujii,⁵ G Panaccione,⁵ M Gorgoi,⁶ J Minar,⁷ J Braun,⁷ H Ebert,⁷ L Plucinski,⁸ OD Dubon,^{1,2} CS Fadley^{1,3}

¹Materials Sciences Division, LBNL, Berkeley, CA, United States; ²Department of Materials Science and Engineering, University of California, Berkeley, CA, United States; ³Department of Physics, University of California, Davis, CA, United States; ⁴National Institute for Materials Science, SPring-8, Hyogo, Japan; ⁵Laboratorio TASC-INFM-CNR, Trieste, Italy; ⁶Helmholtz Center Berlin-BESSY, Berlin, Germany; ⁷Department of Chemistry and Biochemistry, Physical Chemistry Institute, Ludwig Maximilian University, Munich, Germany; ⁸Institute of Solid State Research IFF-9, Research Center Jülich, Jülich, Germany

We used hard angle-resolved X-ray photoemission spectroscopy (ARPES) to investigate the electronic properties of ferromagnetic Ga_{1-x}Mn_xAs as compared to those of pure GaAs, measuring in detail both core-level spectra and angle-resolved valence-band spectra. Data were obtained at both BESSY and SPring-8. The Ga_{1-x}Mn_xAs sample was synthesized by ion implantation and pulsed-laser melting. The measurements were performed at excitation energy of 3.2 eV and 6.0 keV, at which the IMFP of Ga_{1-x}Mn_xAs is ~55-95 Å, making the measurement ~10-20 times more bulk-sensitive compared to traditional soft X-ray photoemission spectroscopy. Core-level multiplet splittings and screening satellites permit better defining the bulk electronic structure. Distinct differences are also found between band structure measurement for Ga_{1-x}Mn_xAs and GaAs. The experimental results will be compared to "one-step model" calculations for photoemission.

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2P096

Hard X-ray photoemission measurement of the band gap in an epitaxial, semiconducting $\text{Cr}_{0.80}\text{Al}_{0.20}$ thin film

Z Boekelheide,^{1,2} AX Gray,^{2,3} DA Stewart,⁴ C Papp,^{2,5} B Balke,^{2,6} S Ueda,⁷ K Kobayashi,⁷ F Hellman,^{1,2} CS Fadley^{2,3}

¹Department of Physics, University of California, Berkeley, CA, United States; ²Material Sciences Division, LBNL, Berkeley, CA, United States; ³Department of Physics, University of California, Davis, CA, United States; ⁴Cornell Nanoscale Facility, Cornell University, Ithaca, NY, United States; ⁵Physical Chemistry II, University of Erlangen, Erlangen, Germany; ⁶Institut für Anorganische und Analytische Chemie, J. Gutenberg-Universität, Mainz, Germany; ⁷NIMS Beamline Station at SPring-8, National Institute for Materials Science, Hyogo, Japan

We have studied an antiferromagnetic $\text{Cr}_{0.80}\text{Al}_{0.20}$ alloy, together with a pure Cr reference sample, with bulk-sensitive hard X-ray photoemission spectroscopy, revealing among other things a semiconducting energy band gap of 85.5 meV (± 13.9 meV). By performing photoemission measurements in the hard X-ray regime, more specifically with the excitation energy of 5956.4 eV, we increase the inelastic mean-free path of the valence-band electrons by a factor of 3-7 compared to conventional soft X-ray photoemission [500 – 1500 eV]. With the ability to probe roughly as far as 25 atomic layers into the sample (using 2.88 Å as the lattice constant for Cr) at 5956.4 eV our measurements become truly bulk-sensitive. Measurements are compared to the theoretical density of states calculations. Core-level spectra are also found to exhibit shifts and satellite effects, and these also will be discussed.

This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

2P097

Hard X-ray photoemission study of $\text{Fe}_{1-x}\text{Si}_x$ binary Heusler alloys

J Karel,¹ AX Gray,^{2,3} C Bordel,⁴ S Ueda,⁵ J Minar,⁶ J Braun,⁶ H Ebert,⁶ K Kobayashi,⁵ F Hellman,^{1,4} CS Fadley^{2,3}

¹Department of Materials Science and Engineering, University of California, Berkeley, CA, United States; ²Department of Physics, University of California, Davis, CA, United States;

³Material Sciences Division, LBNL, Berkeley, CA, United States; ⁴Department of Physics, University of California, Berkeley, CA, United States; ⁵National Institute for Materials Science, SPring-8, Hyogo, Japan; ⁶Department of Chemistry and Biochemistry, Physical Chemistry Institute, Ludwig Maximilian University, Munich, Germany

We used hard X-ray photoemission spectroscopy to investigate the electronic properties of crystalline and amorphous $\text{Fe}_{1-x}\text{Si}_x$ with $x = 0.22$ and 0.35 . These alloys are considered to be binary Heusler alloys, with theory predicting significant spin polarization at the Fermi energy. Films in this composition range can be grown metastably in the bcc structure, thus allowing the effect of composition changes to be studied without a change in crystal structure. By performing photoemission measurements in the hard X-ray regime, more specifically with an excitation energy of 5956.4 eV, we increase the IMFP of valence electrons by a factor of 4 – 7 for these $\text{Fe}_{1-x}\text{Si}_x$ films, with a new IMFP of ~ 76 Å, compared to IMFPs of 11 – 18 Å in the soft X-ray regime of 500 – 1000 eV. The shapes and positions of Si (1s, 2s, 2p) and Fe (2p, 3s, 3p) core levels were investigated for the two compositions ($x = 0.22$ and 0.35) for both crystalline and amorphous samples. Analysis of the valence bands, dominated by Fe 4s, Si 3s and Fe 3d levels revealed significant differences between the compounds of the two compositions and degrees of crystallinity. Our valence band results will also be compared to local density theory, with allowance for matrix element effects.

This work was supported by the U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

2P098

Electronic properties of LaNiO_3 Mott interfaces via hard X-ray photoemission

AX Gray,^{1,2} J Son,³ J M LeBeau,³ S Ueda,⁴ Y Yamashita,⁴ C J Powell,⁵ S Stemmer,³ CS Fadley^{1,2}

¹Department of Physics, University of California, Davis, CA, United States; ²Material Sciences Division, LBNL, Berkeley, CA, United States;

³Materials Department, University of California, Santa Barbara, CA, United States; ⁴National Institute for Materials Science, SPring-8, Hyogo, Japan;

⁵Surface and Microanalysis Science Division, National Institute of Standards and Technology, Gaithersburg, MD, United States

Using core-level hard X-ray photoemission spectroscopy, in conjunction with high-resolution transmission electron microscopy, we have accurately determined effective photoelectron attenuation lengths in epitaxial LaNiO_3 thin films deposited on LaAlO_3 and $(\text{La,Sr})(\text{Al,Ta})\text{O}_3$ substrates. Using these experimentally-determined values, we have then decompose the valence-band spectra of $\text{LaNiO}_3/\text{LaAlO}_3$ and $\text{LaNiO}_3/(\text{La,Sr})(\text{Al,Ta})\text{O}_3$ heterostructures measured in hard X-ray regime into isolated substrate- and thin-film density of states (DOS) components. The resultant thin-film LaNiO_3 densities of states are compared for various thicknesses and substrate materials. Significant differences in the spectral weights are observed for the thinnest epitaxial films. Gap opening, consistent with strain-induced metal-to-insulator transition is observed for the thinnest (2.7 nm) LaNiO_3 film on $(\text{La,Sr})(\text{Al,Ta})\text{O}_3$ substrate.

This work was supported by the ARO MURI Grant W911-NF-09-1-0398

2P099

Bulk electronic structure and recoil effects in LaB_6 via hard X-ray photoemission and hard X-ray ARPES

S Ueda,¹ AX Gray,^{2,3} Y Yamashita,¹ K Kobayashi,¹ CS Fadley^{2,3}¹National Institute for Materials Science, SPring-8, Hyogo, Japan; ²Department of Physics, University of California, Davis, CA, United States; ³Materials Sciences Division, LBNL, Berkeley, CA, United States

We have investigated the bulk electronic structure of LaB_6 using hard X-ray photoemission, measuring in detail both core-level spectra and angle-resolved valence-band spectra. The measurements were performed at the national synchrotron radiation facility SPring-8 in Japan, at undulator beamline 15XU, with photon energies of 5950.26 eV and 3238.12 eV. Binding energy shifts of different magnitudes for the two photon energies were observed in B 1s core peaks due to the recoil effect, a phenomenon in which photoelectrons emitted from a lighter element lose kinetic energy to the atomic nucleus in accordance with the conservation of momentum. The recoil effect, negligible in the soft X-ray regime, becomes prominent at higher kinetic energies, especially for lighter elements, such as boron [atomic mass 10.8]. For Lanthanum, with the atomic mass of 138.9, the recoil effect is still negligible, even at the kinetic energy of 5956.4 eV. Our measurements also revealed the bulk-sensitive band structure of LaB_6 via hard X-ray angle-resolved photoemission [HARPES]. The widely used TPP-2M formula which yields the values of IMFP for most solids predicts IMFPs of 85.55 Å and 51.65 Å for the photoemitted electrons with kinetic energies of 5950.26 eV and 3238.12 eV respectively, thus yielding truly bulk-sensitive measurements of the electronic structure.

This work was funded by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

2P100

Hard X-ray photoelectron spectroscopy at PETRA III

W Drube,¹ S Thiess,¹ A Gloskovskij,² G Berner,³ M Sing,³ G Fecher,² C Felser,² R Claessen³¹Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; ²Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, Mainz, Germany; ³Experimentelle Physik 4, Universität Würzburg, Würzburg, Germany

The well-known strengths of photoelectron spectroscopy for electronic structure investigation at surfaces can effectively be extended to also study complex bulk materials and buried interfaces if hard X-ray excitation is used to increase the electron inelastic mean free path. At third generation synchrotrons this rapidly emerging technique [HAXPES] uses tunable X-rays in the range from about 2 to 15 keV to probe the electronic and chemical structure down to a depth of typically 10-20 nm. A dedicated high resolution HAXPES instrument is currently being commissioned at undulator beamline P09 of the new 6 GeV PETRA III storage ring at DESY (Germany), the most brilliant storage ring source world wide. Good energy resolution down to 100 meV is already obtained from the high heatload primary monochromator which may be further improved by using a double channelcut postmonochromator. In addition, variable linear and circular polarization can be generated by a diamond phase retarder. A set of different mirrors allows focusing down to about 2 x 2 microns on the sample. Photoelectrons up to 15 keV kinetic energy are measured with a SPECS Phoibos 225 HV analyser. First experiments have been done very recently and selected results will be shown.

2P101

Soft-X-ray ARPES endstation at the ADRESS beamline of Swiss Light Source

VN Strocov,¹ T Schmitt,¹ C Hess,¹ X Wang,¹ L Patthey¹¹Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

ARPES experiments in the soft-X-ray energy range bring advantages of free-electron final states, simplified matrix elements and increasing photoelectron escape depth λ . The latter, along with enhancement of the bulk sensitivity, implies improvement of the intrinsic resolution in surface-perpendicular momentum $\Delta k_z = \lambda^{-1}$. In combination with the free-electron final states, this enables reliable investigations of electronic structure in 3-dimensional materials. The ADRESS beamline delivers soft-X-ray photons with circular and 0-180° rotatable linear polarizations in the energy range 300-1600 eV. The ultimate resolution is better than 30 meV at 1 keV photon energy. Intense photon flux up to 1×10^{13} photons/s/0.01%BW at 1 keV helps the problem of small photoexcitation crosssection in the soft-X-ray energy range. The ARPES endstation uses an experimental geometry with 20° grazing light incidence angle to increase the photoyield. The manipulator has three angular degrees of freedom (polar, azimuth and tilt) and is mounted horizontally to balance the light footprint. The analyser (SPECS) is rotatable around the lens axis, which permits the slit orientation either along the beam to exploit symmetry of the valence states, or perpendicular to effectively sample the \mathbf{k} -space. The detection efficiency is characterized by measurements of the Fermi step on gold at 1 keV, which show good statistics within less than 1 min of acquisition.

2P102

Plasma based XUV sources and solutions: synchrotron beamline and endstations supplement for the lab

A Farazahdi,¹ R Lebert,¹ U Wiesemann,¹ W Diete,¹ K Bergmann,² M Benk²

¹Bruker Advanced Supercon GmbH, Bergisch-Gladbach, Germany; ²Fraunhofer Institute for Laser Technology, Aachen, Germany

Strongly supported by the enormous efforts invested in the development of components for EUV Lithography (around 13.5 nm wavelength), the XUV spectral range (1-20 nm, resp. 50 – 1000 eV) has become a fully accessible wavelength range for stand-alone laboratory applications. XUV is of special interest because absorption by photo-effect ionization dominates strongly over scattering, which gives ideal access to elemental and chemical information with cross sections of photon – matter interactions of up to 106 barns also on nano-scale dimensions. Dissemination of successful research from beamlines at storage rings to broader use, however, depends critically on the availability of stand-alone sources. Our plasma emission based XUV-sources have been tuned and integrated into experimental stations such as to approach the quality of beamline installations. This regards average photon flux and intensity, spectral distribution and stability. While availability, uptime and cost aspects may be of high interest, each application requires special solution tailoring, which is within our experience from both synchrotron beamline and laboratory EUV tool developments in the past. We present the scope of XUV laboratory sources ranging from 1 mW/sr to > 10 W/sr (108-1011 photons/s/mrad²) photon flux for quasi-cw spectral broadband emitters over quasi-monochromatic single resonance high brightness line emitters with > 1010 photons/s/mrad²/mm²/0.1% BW. For giving an impression of the potential, we present accomplished dedicated developments for applications, in areas like EUV-Lithography, X-ray and XUV Microscopy (Nanoscopy) and advanced sensitive metrology for analytics of thin film stacks or nanostructures (Nanolitics). With the established concepts of XUV sources the platform for fulfilling many of the demands is available and has proven the reliability and feasibility in a variety of installations world wide.

2P103

Progress in multilayer XUV reflecting Bragg optics

F Bijkerk^{1,2}

¹FOM Institute for Plasma Physics Rijnhuizen, Nieuwegein, Netherlands; ²University of Twente, Enschede, Netherlands

Multilayer reflective elements have been exploited in the XUV spectral range ever since the early seventies [i], but only lately have they experienced a major boost in optical performance [ii]. This has been a result of an extended, industry-driven research effort for a most demanding optical application, namely diffraction-limited imaging at a wavelength of 13 nm: EUV lithography. Deposition technologies now allow multilayer performances of over 95% of the theoretical reflectivities, achieved by controlling the chemical interface processes and by lowering the interface roughness. New optical configurations include combinations of multilayer Bragg systems with lateral Fresnel grating structures, which are shown to suppress undesired non-specular wavelengths or enhance the monochromaticity [iii], [iv]. Other examples include adaptive properties that allow a variation of the multilayer periodicity, and thus the possibility to tune the reflected wavelength. Essentially, these optical possibilities can be now considered for new or optimized applications in science and technology, like for X-ray free electron lasers, requiring high-stability multilayers, and high brightness synchrotron beam lines. The presentation will include an overview of the technological capabilities as well as the new optical insight gained by this optics research.

[i] E. Spiller, SPIE Press, Bellingham, 1994.

[ii] A.E. Yakshin, R.W.E. van de Kruijs, et al., Proc. SPIE 6517-17 (2007).

[iii] V.V. Aristov, A.I. Erko, Moscow, Pub. Nauka, 1991.

[iv] R. van der Meer, I. Kozhevnikov, et al., EOS Diffractive Optics 2010.

TUESDAY PROGRAM

3PL Theory & computation

Chair: Eric Shirley

9:00 - 10:10

LIFE SCIENCES INSTITUTE 2

3PL1 John Rehr (plenary)

9:00 Full-spectrum calculations of optical response from UV-Vis to X-rays

3PL2 Hubert Ebert (invited)

9:40 Calculation of angle-resolved photoemission spectra within the one-step model of photo emission - recent developments

Coffee

10:10 - 10:40

3A Dynamics (1)

Chair: Kiyushi Ueda

10:40 - 12:30

LIFE SCIENCES INSTITUTE 2

3A1 Alexander Föhlisch (invited)

10:40 Transient phases and phase transitions probed with ultrafast X-ray scattering and spectroscopy

3A2 Kai Rossnagel

11:10 Femtosecond time-resolved photoemission of layered charge-density-wave compounds

3A3 Yuhai Jiang

11:30 Investigating two-photon double ionization of D_2 by XUV pump-probe experiments at FLASH

3A4 Roman Adam

11:50 Measurement of demagnetization dynamics at the M edges of Ni and Fe using a tabletop high-harmonic soft X-ray source

3A5 He Wang

12:10 Attosecond XUV transient absorption spectroscopy

3B Correlated electron systems

Chair: Wendy Flavell

10:40 - 12:30

FOREST SCIENCES 1005

3B1 Amina Taleb-Ibrahimi (invited)

10:40 Novel electronic properties of layered compounds and tunnel junctions: prospects for superconductivity and magnetism

3B2 Hideaki Iwasawa

11:10 Polarization and kz-dependent ARPES study of Sr_2RuO_4

3B3 Kenya Shimada

11:30 High-resolution ARPES study of many-body interactions in metals

3B4 Andrea Damascelli (invited)

11:50 - 12:20 ARPES on correlated and superconducting oxides

Lunch

12:30 CONFERENCE PHOTO

12:30 - 14:00

POSTER SESSION 3P

Chair: Yongfeng Hu

EAST AND WEST ATRIA, LIFE SCIENCES CENTRE

14:00 - 15:40

3C Liquids and in situ studies

Chair: Nobuhiro Kosugi

16:00 - 18:00

LIFE SCIENCES INSTITUTE 2

3C1 Emad Flear Aziz (invited)

16:00 Charge transfer to solvent identified via dark channel fluorescence yield L-edge spectroscopy

3C2 Monika Blum

16:30 The electronic structure of amino acids in aqueous solution studied by soft X-ray spectroscopy

3C3 Franz Hennies

16:50 Vibrational soft X-ray Raman scattering of liquids and gases

3C4 Kathrin Maria Lange

17:10 The hydrogen bond character of water in solvents of different polarity

3C5 Tony Van Buuren

17:30 In-situ X-ray spectroscopy for investigation of advanced materials for electrical energy storage (EES)

3D Electron spectroscopies

Chair: Steve Kevan

16:00 - 18:00

FOREST SCIENCES 1005

3D1 Donglai Feng (invited)

16:00 Unconventional spin density waves in iron-based superconductors and their parent compounds

3D2 Kaoru Iwano

16:30 Domain excitation as a novel type of electron excitation: manifestations in ARPES and IXS

3D3 Giorgio Levy

16:50 Doping evolution of zero-energy excitations in high-Tc superconductors as observed by ARPES

3D4 Markus Donath

17:10 Spin-dependent surface states on Co/Cu(001): sensors for surface roughness and surface alloying

3D5 Joerg Osterwalder (invited)

17:30 - 18:00 Surface states as a bonanza for spin-polarized electrons

3PL3

SPECIAL PUBLIC LECTURE

Paul Corkum: Catching electrons with light?

20:00 - 21:00

LIFE SCIENCES INSTITUTE 2

3PL1

Full-spectrum calculations of optical response from UV-Vis to X-rays

John J. Rehr¹ E.L. Shirley,² J. Vinson,¹ J.J. Kas¹ and H.M. Lawler¹

¹ Dept. of Physics, Univ. of Washington, Seattle, WA, USA.

² Natl. Inst. of Standards and Technology, Gaithersburg, MD, USA.

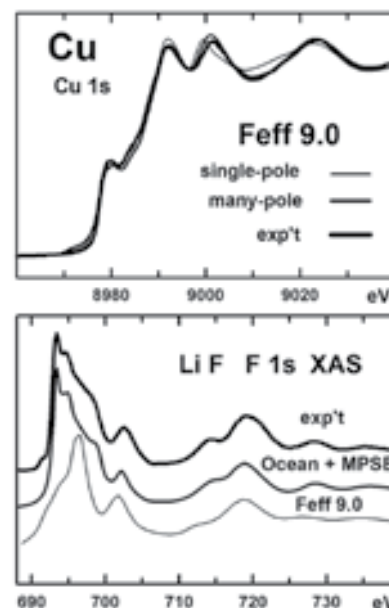
There has been dramatic progress in recent years in theories of optical and electron-spectroscopies. This progress has been spurred by advances in the treatment of several key many-body effects, namely particle-hole interactions, inelastic losses, and Debye-Waller factors. Here we review two complementary approaches: First is an approach based on real-space Green's function (RSGF) code FEFF9 [1]. Second is a reciprocal-space approach based on the GW/Bethe-Salpeter Equation (GW/BSE) [2]. For core-excitations the quasi-particle theory in FEFF9 is equivalent to that in the GW/BSE. To improve on phenomenological models, FEFF9 uses parameter free treatments of the key many-body effects, including a many-pole GW self-energy (MPSE) to treat inelastic losses. Our GW/BSE approach is implemented in two hybrid codes: OCEAN (Obtaining Core Excitation using ABINIT and NBSE) for core-spectra and AI2NBSE for valence spectra [3]. Both codes use pseudopotential wavefunctions from a plane-wave code (e.g. ABINIT), the NIST BSE solver, and the same MPSE. Each has its advantages and disadvantages. For example, AI2NBSE and OCEAN have limited spectral ranges and require a supercell to treat aperiodic systems, while FEFF9 is applicable over a broad spectrum but less accurate near an edge. However, combining both methods now permits accurate full spectrum calculations of photon and electron spectroscopies from the UV-Vis to X-ray energies.

*Supported by DOE Grant DE-FG03-97ER45623, and facilitated by the DOE CMSN.

[1] J. J. Rehr et al., *Comptes Rendus Physique* 10, 548 [2009].

[2] G. Onida et al., *Rev. Mod. Phys.* 74, 601 [2002].

[3] H. Lawler et al., *Phys. Rev. B* 78, 205108 [2008]; J. Vinson, et al UW Preprint [2010].



John Rehr received a Ph.D. in Theoretical Condensed Matter Physics from Cornell University in 1972 working with Prof. N. D. Mermin. A NATO postdoctoral fellowship at King's College London (1972-73), and a postdoctoral appointment with Prof. W. Kohn at University of California, San Diego, (1973-1975) followed. In 1975, Prof. Rehr joined the Department of Physics at the University of Washington. Prof. Rehr has held visiting appointments at Cornell University (1986-88) working with Prof. K. Wilson, and at Lund University (spring 1994) with Prof. Lars Hedin. Prof. Rehr is also a Consulting Professor at the Stanford Synchrotron Radiation Lightsource, Co-coordinator of the DOE Computational Materials Science Network, and head of the Theoretical X-ray Beamline of the European Theoretical Spectroscopy Facility (ETSF). Prof. Rehr's research specialties are in condensed matter theory, with major interests in excited state electronic structure and the theory of X-ray and electron spectra. His group is especially known for the development of quantitative theories of EXAFS and other core-level X-ray and electron spectroscopies, as implemented in the FEFF codes.

3PL2 (Invited)**Calculation of angle-resolved photo emission spectra within the one-step model of photo emission - recent developments**H Ebert,¹ J Minar,¹ J Braun,¹ S Mankovsky¹¹University Munich, Dept. Chemistry, Munich, Germany

Various technical developments enlarged the potential of angle-resolved photo-emission (ARPES) tremendously during the last one or two decades. In particular improved momentum and energy resolution as well as the use of photon energies from few eV up to several keV makes ARPES a rather unique tool to investigate the electronic properties of solids and surfaces. Obviously, this rises the need for a corresponding theoretical formalism that allows to accompany experimental ARPES studies in an adequate way. As will be demonstrated by several examples this goal could be achieved by various recent developments on the basis of the one-step model of photo-emission: The spin-orbit induced Rashba-splitting of Shockley-type surface states is discussed using a fully relativistic description. The impact of chemical disorder within surface layers can be handled by means of the Coherent Potential Approximation (CPA) alloy theory. Calculating phonon properties together with the corresponding electron-phonon self-energy allows a direct comparison with features in the ARPES spectra caused by electron-phonon interaction. The same holds for the influence of electronic correlation effects. These are accounted for by means of the dynamical mean field theory (DMFT) that removes the most serious shortcomings of standard calculations based on the plain local density approximation (LDA). The combination of this approach with the CPA allows the investigation of correlated transition metal alloys. Finally, accounting for the photon momentum and going beyond the single scatter approximation for the final state allows to deal quantitatively with ARPES in the high-energy regime (HAXPES) that reduces the influence of the surface on the spectra and probing primarily the bulk electronic structure this way. Corresponding calculations of ARPES spectra, however, have to deal with thermal vibrations in an adequate way. For this, a new scheme is suggested that makes use of the CPA.

LIFE SCIENCES INSTITUTE 2

10:40-12:30

3A1 (Invited)**Transient phases and phase transitions probed with ultrafast X-ray scattering and spectroscopy**A Föhlisch¹¹Institute for Methods and Instrumentation in Synchrotron Radiation Research G-12 Helmholtz-Zentrum Berlin, Berlin, Germany;²Institut für Physik und Astronomie Universität Potsdam Karl-Liebknecht-Strasse 24-25, Potsdam, Germany

In materials science and femtochemistry, the frontier of knowledge spans from molecular surface dynamics for heterogeneous catalysis with little explored transition states to functional materials with often surprising properties and phase transitions as well as to chemical dynamics in solution. In these systems the interplay between local properties and nanoscale phenomena govern their physics and chemistry - and femtosecond soft X-ray pulses are ideal probes of their dynamics. With innovative X-ray sources first steps into femtosecond time resolved X-ray methods have been taken and the new physics we can access is explored through our research of femtosecond time resolved X-ray scattering and spectroscopy for materials science.

3A2

Femtosecond time-resolved photoemission of layered charge-density-wave compounds

K Rossnagel,¹ S Hellmann,¹ C Sohr,¹ M Kalläne,¹ L Kipp,¹ M Beye,² F Sorgenfrei,² A Föhlisch,^{2,3} W Wurth,² T Rohwer,¹ M Wiesenmayer,¹ M Bauer¹

¹University of Kiel, Kiel, Germany; ²University of Hamburg, Hamburg, Germany; ³Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Charge-density waves (CDWs) are broken-symmetry states of low-dimensional solids that are brought about by electron-phonon interaction. Yet, surprisingly, a clear microscopic understanding beyond this statement has not emerged for two-dimensional systems. Here, we will look at this classical paradigm of condensed matter physics with femtosecond time-resolved photoelectron spectroscopy using pulsed extreme ultraviolet radiation generated by a free-electron laser (FLASH) and a high-harmonic-generation source in Kiel. We will restrict ourselves to CDWs in two layer compounds, in the Mott insulator 1T-TaS₂ and in the possible excitonic insulator 1T-TiSe₂. We will determine how fast a CDW can melt and how fast it approaches equilibrium after impulsive optical excitation and we will particularly investigate whether the ultrafast vaporization and equilibration dynamics provides a key to the origin of CDWs in two dimensions.

3A3

Investigating two-photon double ionization of D₂ by XUV pump-probe experiments at FLASH

YH Jiang,¹ A Rudenko,² J F Pérez-Torres,³ O Herrwerth,⁴ L Foucar,² M Kurka,¹ KU Kühnel,¹ E Plésiat,³ F Morales,³ F Martín,³ M Lezius,⁴ M Kling,⁴ T Jahnke,⁵ R Dörner,⁵ JV Tilborg,⁶ A Belkacem,⁶ M Schulz,⁷ K Ueda,⁸ TJM Zouros,⁹ S Düsterer,¹⁰ R Treusch,¹⁰ CD Schröter,¹ R Moshhammer,¹ J Ullrich¹

¹Max-Planck-Institut für Kernphysik, Heidelberg, Germany; ²Max-Planck Advanced Study Group at CFEL, Hamburg, Germany; ³Departamento de Química C-9, Madrid, Spain; ⁴Max-Planck-Institut für Quantenoptik, Garching, Germany; ⁵Universität Frankfurt, Frankfurt, Germany; ⁶Lawrence Berkeley National Laboratory, Berkeley, Germany; ⁷Missouri University of Science & Technology Rolla, Rolla, United States; ⁸Tohoku University, Sendai, Japan; ⁹Department of Physics, University of Crete, Crete, Greece; ¹⁰DESY, Hamburg, Germany

Using a novel split-mirror set-up attached to a Reaction Microscope at the Free electron LASer in Hamburg (FLASH) we performed a XUV pump-probe experiment by tracing the ultra-fast nuclear wave-packet motion in the D₂⁺(1sσ_g⁺) with < 10 fs time resolution. Comparison with time-dependent calculations shows excellent agreement with the measured vibrational period of 22 ± 4 fs in D₂⁺, points to the importance of accurately knowing the inter-nuclear distance dependent ionization probability and paves the way to control sequential and non-sequential two-photon double ionization contributions.

3A4

Measurement of demagnetization dynamics at the M edges of Ni and Fe using a tabletop high-harmonic soft X-ray source.

R Adam,¹ P Grychtol,¹ C La-O-Vorakiat,² S Mathias,³ M Siemens,⁴ J Shaw,⁴ H Nembach,⁴ T Silva,⁴ M Aeschlimann,³ CM Schneider,¹ HC Kapteyn,² MM Murnane²

¹Institute of Solid State Research, Research Centre Juelich, Juelich, Germany; ²Department of Physics and JILA, University of Colorado, Boulder, United States; ³TU Kaiserslautern and Research Centre OPTIMAS, Kaiserslautern, Germany; ⁴Electromagnetics Division, National Institute of Standards and Technology, Boulder, United States

Pump-probe measurements based on ultrafast pulsed lasers have been the technique of choice to test the magnetization dynamics with femtosecond temporal resolution. On the other hand, static soft X-ray experiments at the synchrotron showed that the magnetization can be probed element-selectively by tuning the probe-beam energy to the M absorption edges of Fe, Co, and Ni. Recently, newly developed soft X-ray sources based on the high-harmonic up-conversion of ultrafast pulsed lasers promise to combine femtosecond temporal resolution with element-selectivity in the single tabletop experiment. Our experiment was set up in a transverse magneto-optic Kerr effect geometry. Reflecting laser-generated X-ray pulses off a magnetized NiFe grating large magneto-optic signal of up to 6% at the M absorption edges of Fe and Ni were observed. In our pump-probe experiment, short laser pump pulses were first directed at the sample to destroy the magnetic order. Inherently synchronized X-ray probe pulses were then reflected from the targeted spot to measure the element-specific demagnetization. Our results show a strong NiFe magnetization reduction within 400 fs after the pump beam excitation and point towards a strong coupling of the magnetic moments of Ni and Fe forming the NiFe film.

3A5

Attosecond XUV transient absorption spectroscopy

H Wang,¹ M Chini,¹ S Chen,¹ Z Chang¹

¹J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan/Kansas, United States

Time-resolved X-ray absorption spectroscopy has been demonstrated to be a powerful tool for studying phase transitions. However, the time resolution is limited to picosecond or femtosecond at synchrotron facilities. We have developed an experimental setup for conducting XUV/x-ray absorption with attosecond precision. Using the double optical gating method, which is a combination of polarization gating and two-color gating, a smooth continuous spectrum covering 20 eV to 600 eV was produced with 8 fs, ~1 mJ lasers centered at 800 nm operating at 1 kHz. The duration of the XUV pulse can be as short as 110 as. The setup consists of three parts. The first one is the XUV generation chamber, where the laser pulse with a time-dependent ellipticity is focused on a gas target. The type of gases used depends on the applications. For example, Xe gas is suitable for generating intense attosecond pulses in the 20 to 30 eV photon energy range. The XUV beam is focused to the sample in the second chamber with a toroidal mirror at grazing incidence. Gas samples have been studied so far, but other types of samples can also be investigated. The XUV beam size on the sample is ~30 μm. A portion of the 800 nm laser pulse is also focused on the sample, which is temporally and spatially overlapped with the XUV pulse. The intensity of the laser beam can reach 10¹⁴ W/cm². A CW green laser co-propagates with the XUV and laser beam to stabilize the path length difference between the two beams. The delay between the XUV pulse and the laser field can be adjusted with 22 as precision. The transmitted XUV beam was measured with a transmission grating (2000 lines/mm or 5000 lines/mm) spectrometer. The spectrum is recorded on a MCP imager and CCD camera. The spectrometer resolution is better than 80 meV at 30 eV. In time-resolved experiments, the XUV spectrum is measured as a function of the delay between the XUV and NIR pulses. The attosecond dynamics of Fano resonances of noble gas was studied experimentally using this setup.

3B1 (Invited)**Novel electronic properties of layered compounds and tunnel junctions : prospects for superconductivity and magnetism**A Taleb-Ibrahimi¹¹CNRS/Synchrotron SOLEIL, Gif/Yvette, France

Materials with exotic properties, like thermoelectricity, high temperature superconductivity, giant magnetoresistance have attracted large interest recently. In this lecture we will report on angle and spin resolved photoemission investigations, using the high performances of the new Cassiopée beamline at Soleil, which reveals novel electronic and magnetic signatures in advanced materials. The case of misfit cobaltates [1] or the newly discovered pnictides superconductors [2] demonstrates the role of many body interactions responsible for the exotic physical properties of these highly correlated systems. Electrons correlations are also present in low dimensional systems as the alkali/Si(111) Mott insulator which exhibits a phase transition consistent with the possible formation of a bipolaronic phase at the surface with triangular geometry with alternating doubly occupied and unoccupied bonds as expected in the Holstein-Hubbard model [3]. This case illustrates the competition between e-e correlations and e-phonon coupling at a surface. Improving magnetic tunnel junctions-MTJs (larger magnetoresistance-TMR) remains a major challenge for technological developments. MgO-based epitaxial MTJs as studied by Spin polarized X-ray Photoemission show electronic states responsible for increased TMR. These investigations are a step forward in the understanding of the tunnel transport in these type of junctions [4]. Tailoring and modelizing novel electronic states is challenging for the fundamental physics as well as of great interest for future technological applications.

[1] A. Nicolaou et al PRL 103, 2009, EPL 2010, [2] V. Brouet et al PRB 80, 2009 and arXiv :1002.4952, [3] Luis Cardenas PhD Thesis, 2010, [4] F. Bonell et al IEE Trans. on Magn., 10, 2009.

3B2**Polarization and k_z -dependent ARPES study of Sr_2RuO_4** H Iwasawa,¹ Y Yoshida,² I Hase,² H Hayashi,³ J Jiang,³ K Shimada,¹ H Namatame,¹ M Taniguchi,^{1,3} Y Aiura²

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; ³Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan

The monolayer ruthenate Sr_2RuO_4 has attracted considerable attentions for number of reasons such as unconventional superconductivity, a structural similarity to the cuprates, and a two-dimensional Fermi liquid behavior in the normal states. Furthermore, the multiband near- E_F electronic structure is essential feature of Sr_2RuO_4 , which is contrast to the cuprates possessing a single band. Our previous high-resolution ARPES studies of Sr_2RuO_4 clarified an existence of the kink structure and orbital dependence of the magnitude of the kink [1, 2]; a kink was clearly observed for the γ band derived from the d_{xy} orbital, while not for the α and β bands derived from the d_{yz} and d_{zx} orbitals. However, it was difficult to get the precise band dispersion especially in the high-energy region because these bands are located closely. To overcome this difficulty, we have performed the polarization and photon-energy dependent ARPES study of Sr_2RuO_4 . The high-resolution ARPES data were measured at a newly developed rotatable high-resolution ARPES system on BL-1 at Hiroshima Synchrotron Radiation Center. By tuning the photon-energy and the polarization, we can selectively observe a specific band, giving us an opportunity to get a new insight into the band structure. Here, we will discuss the orbital dependent mass enhancement of Sr_2RuO_4 in view of both electronic and bosonic origins.

[1] Y. Aiura *et al.*, Phys. Rev. Lett. **93** 117005 (2004).

[2] H. Iwasawa *et al.*, Phys. Rev. B. **72** 104514 (2005).

3B3

High-resolution ARPES study of many-body interactions in metals

K Shimada,¹ J Jiang,² XY Cui,³ H Hayashi,² D Hirayama,² H Iwasawa,¹ M Arita,¹ Y Aiura,⁴ H Namatame,¹ M Taniguchi¹

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ³Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland; ⁴National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

High-resolution angle-resolved photoelectron spectroscopy (ARPES) in the VUV and soft X-ray range enables us to elucidate bulk- and surface-derived energy-band dispersions and Fermi surfaces in detail. In this presentation, we report high-resolution ARPES study of metals (Ni, Cu, Al, and Fe) and clarify magnitudes of the many-body interactions on the quasi-particles near the Fermi level. All of the high-resolution ARPES experiments were performed on the undulator beamlines (BL-1 and BL-9A) of a compact electron-storage ring (HiSOR) at Hiroshima University. We have observed a kink structure derived from the electron-phonon interaction in the energy-band dispersion. Based on the quantitative lineshape analyses, we have experimentally obtained real and imaginary parts of the self-energy. The coupling parameters of the electron-phonon and electron-electron interactions were evaluated. We will compare and discuss magnitudes of the parameters in these metals.

3B4 (Invited)

ARPES on correlated and superconducting oxides

A Damascelli¹

¹University of British Columbia, Vancouver, BC, Canada

In this talk I will review our studies of correlated and superconducting oxides, such as the p-wave superconductor Sr_2RuO_4 and the high-Tc cuprates, by a combination of ARPES and density functional theory. For Sr_2RuO_4 this reveals subtle yet important details of the band structures, such as the mixing of orbital character and spin anisotropy induced by spin-orbit interaction, which might have direct implications for the elusive pairing mechanism. In the cuprates, by means of the in-situ doping approach, we have been able to obtain a quantitative estimate of the quasiparticle integrity Z from the more conventional heavily overdoped ($p \sim 0.40$) to the correlated deeply underdoped ($p \sim 0.02$) regime. While a remarkable agreement with the $Z = 2p/(p+1)$ meanfield predictions is found at large doping, we observe the breakdown of the quasiparticle pictures at $p \sim 0.10$ - 0.15 . This defines the boundary for the crossover from Fermi-liquid to Mott physics.

3C1 (Invited)**Charge transfer to solvent identified via dark channel fluorescence yield
L-edge spectroscopy****EF Aziz,¹ MH Rittmann-Frank,^{1,2} KM Lange,¹ S Bonhommeau,³ M Chergui²**¹Helmholtz Zentrum Berlin, Berlin, Germany; ²EPFL, Lausanne, Switzerland; ³CNRS, Toulouse, France

Aqueous ions are central to catalysis and biological function and play an important role in radiation biology as sources of electrons that may induce subsequent damage. Detailed knowledge about the solute-solvent interaction is therefore crucial. For transition metal ions, soft X-ray L-edge spectroscopy allows one to access the *d*-orbitals, which are those directly interacting with the solvent molecules. Here we show that fluorescence yield spectra of aqueous ionic species exhibit spectral features that lie below the fluorescence background from the solvent. These features are rationalised as a competition between the fluorescence yields of the solute and solvent species, and between the solute radiative (fluorescence) and non-radiative channels, such as electron transfer to the water molecules. We can thus determine the nature, directionality and time scale of the charge transfer. Remarkably, even in the case of fully ligand-coordinated ions we do observe electron transfer to the water molecules.

3C2**The electronic structure of amino acids in aqueous solution studied by
soft X-ray spectroscopy****M Blum,^{1,2} M Odelius,³ L Weinhardt,² S Pookpanratana,¹ M Bär,⁴ Y Zhang,¹ O Fuchs,² JD Denlinger,⁵ W Yang,⁵ E Umbach,⁶
C Heske¹**¹Department of Chemistry, University of Nevada Las Vegas, Las Vegas, United States; ²Experimentelle Physik VII, Universität Würzburg, Würzburg, Germany; ³FYSIKUM, Stockholm University, Stockholm, Sweden; ⁴Solar Energy Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; ⁵Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, United States; ⁶Karlsruhe Institute of Technology, Karlsruhe, Germany

Recently, soft X-ray emission (XES) and absorption (XAS) spectroscopy have been employed to probe the electronic structure of liquids. Such experiments represent a technically challenging task. Using a custom-built experimental endstation (SALSA), which includes a novel liquid flow-through cell and a high-efficiency X-ray spectrometer, we have investigated the electronic structure of various liquids and aqueous solutions under well-defined and reproducible experimental conditions. We will present 2-dim. resonant inelastic X-ray scattering (RIXS) maps of amino acids in aqueous solution at different pH-values. Such RIXS maps reveal unprecedented details of the electronic structure of solids and liquids. Our investigation of aqueous amino acid solutions shows that the local electronic structure changes significantly upon protonation or deprotonation of the different functional groups. For solutions with different pH-values, the spectra show a strong variation in peak intensity, which is explained by ultra-fast proton dynamics on the time scale of the core hole lifetime, and give a distinct spectral signature for the functional groups of the amino acid solution. A model, supported by first principle density functional theory calculations, will also be discussed.

3C3

Vibrational soft X-ray Raman scattering of liquids and gases

F Hennies,^{1,6} Y Sun,² M Odellius,³ M Berglund,^{4,8} A Pietzsch,¹ J Schlappa,⁴ B Kennedy,¹ T Schmitt,⁵ V Strocov,⁵
J Andersson,⁶ H Karlsson,⁷ F Gel'mukhanov,² JE Rubensson,⁵ A Föhlisch^{4,8}

¹MAX-lab, Lund University, Lund, Sweden; ²Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden; ³FYSIKUM, Albanova, Stockholm University, Stockholm, Sweden; ⁴Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ⁵Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland; ⁶Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden; ⁷Department of Physical and Analytical Chemistry, Uppsala, Sweden; ⁸Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

Most fundamental questions regarding the function of complex molecular systems are related to local electronic and dynamic properties of different molecular building blocks. Core-resonant soft X-ray spectroscopy has for a long time allowed access to local electronic structure information, and in recent time its application, in particular when applied in photon-in-photon-out mode, has successfully been extended to the investigation of liquids. However, direct information about local coordination and dynamics, in particular of the ground state, has up to now not been accessible. We have now performed resonant inelastic soft X-ray scattering (RIXS) spectra of liquids (acetone, water) and gases (O₂, CO₂) with a resolution of $E/E \sim 10000$. This is, for the first time, sufficient to resolve single vibrational modes, allowing for a description of the potential energy surfaces of ground state and excited states in unprecedented accuracy. RIXS maps out vibrational modes with element sensitivity in symmetry resolved manner, and can therefore provide information, in particular on the electronic ground state, which no other technique can access. Highly energy resolved spectra obtained at the ADDRESS beamline at the SLS are presented along with ab-initio multimode scattering calculations that resemble the data in very high detail. Influences of molecular interaction in the liquid environment are discussed, along with some new in-sights in the local coordination of liquid water.

3C4

The hydrogen bond character of water in solvents of different polarity

KM Lange,¹ KF Hodeck,¹ MH Rittmann-Frank,^{1,2} U Schade,¹ EF Aziz Bekhit¹

¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ²Ecole Polytechnique Fédérale de Lausanne, Lausanne-Dorigny, Switzerland

X-ray absorption and Fourier transform infrared spectroscopy were used to study the hydrogen bond of isolated water molecules in organic solvents of different polarity in comparison to bulk water. The electronic structure of isolated water molecules shows a more ice-like than gas-like electronic structure. A systematic shift of the σ^* shape resonance towards higher energies is observed upon varying the solvent from chloroform to benzene to acetonitrile, and to water, corresponding to an increase of the hydrogen bond strength, confirming the validity of the "bond-length-with-a-ruler" principle. This observation is supported by shifts of the OH-stretching modes to lower wave numbers respectively. Raising the water concentration induces a solvent specific clustering of the water molecules.

3C5

In-situ X-ray spectroscopy for the investigation of advanced materials for electrical energy storage (EES)

J Lee,¹ T Willey,¹ J Guo,² M Nielsen,² T van Buuren¹

¹Physics and Life Science Division, Lawrence Livermore National Laboratory, Livermore CA, United States; ²Lawrence Berkeley National Laboratory, Berkeley CA, United States; ³Dalhousie University, Halifax NS, Canada

In situ characterization of the evolution in electronic structure of electrode materials during repeated charge-discharge cycling is fundamentally important for more fully understanding the processes of charge storage and degradation, which, in turn, is essential for the development of new electrical energy storage (EES) materials with tailored properties and improved performance. X-ray spectroscopies provide ideal tools with which to obtain enhanced insight into the origins of electrode behavior in EES systems due to their capabilities for direct, element specific, characterization of the electronic densities of states. To date, in situ studies of EES materials have primarily focused on hard X-ray experiments due to the challenges associated with UHV compatibility and high photon attenuation of cells for soft X-ray measurements. Nonetheless, the use of soft X-ray spectroscopies to EES systems is vital since they provide complementary information that cannot be obtained via hard X-ray studies. We report the development of a cell for in situ soft X-ray emission spectroscopy and X-ray absorption spectroscopy studies of EES materials and will discuss experiments focused upon the X-ray spectroscopy characterization of a series of novel electrode materials for application in rechargeable Li-ion batteries. Prepared by LLNL under Contract DE-AC52-07NA27344.

FOREST SCIENCES CENTRE 1005

16:00-18:00

3D1 (Invited)

Unconventional spin density waves in iron-based superconductors and their parent compounds

DL Feng¹

¹Dept. of Physics, Fudan University, Shanghai, China

One intriguing phenomenon in iron-based high-temperature superconductors (Fe-HTSC) and their parent compounds is the spin density wave transition that is accompanied by a structural transition. The ubiquitous appearance of the magnetic and structural transitions in various families of iron-based systems makes it crucial to understand their nature and origin. In the talk, I will present our recent angle resolved photoemission data on the electronic structure of NaFeAs, LaOFeAs, Fe_{1+y}Te, and Ba/Sr/Eu-Fe₂As₂. Our results show that it is the electronic structure reconstruction rather than the Fermi surface nesting that drives both the structural and magnetic transitions in these compounds. Moreover, we show that electron correlations play a very important role, and induce different manifestation of such a mechanism in different compounds.

3D2

Domain excitation as a novel type of electron excitation: manifestations in ARPES and IXS

K Iwano¹¹Photon Factory, Tsukuba, Japan

Heavily renormalized nature of quasi-particles typically seen in the ARPES of strongly-correlated electron systems have collected much attention, since the nature can provide important information on the many-body properties of those systems. However, even in such cases the quasi-particle is basically one particle; the strong renormalization only increases the particle mass and reduces its lifetime. In this paper, we report on a completely different type of excitation that can be detected in the ARPES and IXS [1]. We assume a case where a system that is located close to a phase boundary absorbs one high-energy photon. Assuming valence photoemission, we are left with one hole in the valence band. In ordinary insulators, the process stops at this point. However, in this system, it does not stop but proceeds to form a domain [2]. We here think of a one-dimensional system whose outer electron occupancy is expressed as "... 020202...". TTF-CA, an organic molecular solid, is a system appropriate for this situation, having nearly degenerate neutral (N) and ionic (I) phases. In the process after photoexcitation, we expect that a domain of the I phase is created in the background of the N phase. The detection of this process requires no pump-probe experiment but only an ordinary type of photoemission measurement.

[1] K. Iwano, Phys. Rev. Lett. 102, 106405 (2009).

[2] K. Iwano, Phys. Rev. Lett., 97, 226404 (2006).

3D3

Doping evolution of zero-energy excitations in high- T_c superconductors as observed by ARPES

G Levy,¹ J Rosen,¹ D Fournier,¹ A Bostwick,² E Rotenberg,² Y Yoshida,³ H Eisaki,³ R Liang,¹ W Hardy,¹ D Bonn,¹ IS Elfimov,¹ A Damascelli¹

¹Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada; ²Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, United States; ³National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

The continuous doping evolution from an antiferromagnetic charge-transfer insulator into a record high- T_c superconductor is arguably the most intriguing aspect of the layered cuprates physics. As the antiferromagnetic insulating phase is approached from the superconducting state, angle-resolved photoemission spectroscopy (ARPES) on $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ (YBCO) observes the collapse of the large hole-like Fermi surface into the so-called Fermi arcs - disconnected segments of zero-energy excitations in momentum space [1]. This is in contrast to quantum oscillation experiments, which suggest the existence of a close Fermi surface of well-defined quasiparticles in the underdoped regime [2]. We will discuss the characteristics of the Fermi surface as observed by ARPES in two different materials, YBCO and La-doped $\text{Bi}_2(\text{Sr}_{2-x}\text{La}_x)\text{Cu}_2\text{O}_{6+\delta}$, aiming at establishing a universal picture for the underdoped cuprates and the role of electronic/versus lattice degrees of freedom in possible reconstructions of the Fermi surface.

[1] M.A. Hossain *et al.*, Nature Physics **4**, 527 (2008).[2] N. Dorion-Leyraud *et al.*, Nature **447**, 565 (2007).

3D4

Spin-dependent surface states on Co/Cu(001): sensors for surface roughness and surface alloying

M Donath,¹ T Allmers¹

¹Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Münster, Germany

Ultrathin fcc Co films on Cu(001) are a prototype system in low-dimensional magnetism. The film quality with respect to morphology and alloying is influenced by the growth conditions and has consequences for the magnetic properties. We have combined scanning tunneling microscopy (STM) with spin-resolved direct and inverse photoemission (I)PE to relate the film morphology, observed with STM, with the surface electronic structure, observed with spin-resolved (I)PE. The Co(001) surface exhibits two distinct surface states: an occupied minority d-derived surface state S1 in a symmetry gap around $\bar{\Gamma}$ and an unoccupied exchange-split sp-like surface state S2 around \bar{X} . S1 and S2 are characteristic of the flat and clean surface and react sensitively but, due to their distinct character, differently to changes in surface roughness and composition. Films prepared at low temperature without annealing result in a rough surface, where S2 is absent but S1 appears with reduced intensity. Annealing to temperatures above 555 K causes Cu diffusion to the surface, which results in a suppression of S1. This indicates that the symmetry gap closes for the Co-Cu alloy due to the non-magnetic Cu. In contrast, the projected bulk band structures for Co(001) and Cu(001) are very similar above the Fermi level including the gap position around \bar{X} . Consequently, S2 persists but with a reduced exchange splitting. The same is true for a third surface state, the image-potential state around $\bar{\Gamma}$ below the vacuum level. Our results demonstrate how important a careful film preparation is for the study of well-defined Co films – and how surface states can be used to sensitively monitor the film properties.

3D5 (Invited)

Surface states as a bonanza for spin-polarized electrons

J Osterwalder,¹ F Meier,¹ JH Dil¹

¹Physik-Institut, Universitaet Zuerich, Zuerich, Switzerland

Since the pioneering work of LaShell et al. [1] it is recognized that the spin-orbit interaction in combination with the breaking of spatial inversion symmetry at surfaces can lead to spin-splitting of electronic surface states on metals via the so-called Rashba effect. Some years later the spin polarization resulting from this splitting, as well as the momentum-dependent spin texture, could be measured on Au(111) [2]. In the meantime it appears that spin polarization is a ubiquitous phenomenon in electronic states at or near surfaces. Our group has contributed to this knowledge by means of an angle-resolved photoemission apparatus equipped with a three-dimensional spin polarimeter [3], and by introducing a powerful two-step fitting procedure for deriving three-dimensional spin polarization vectors [4]. Several case studies will be presented. On surface alloys of Bi and Pb on Ag(111) a giant spin splitting leads to a Rashba-type, mostly in-plane spin texture, but a significant out-of-plane component could be detected as well [4]. On a related Sb/Ag(111) surface alloy, a very small spin splitting below the intrinsic line widths leads to a coherent superposition of spin states with a concomitant rotation of their polarization vectors [5]. On vicinal Au(111) surfaces it was demonstrated that the spin polarization and the helical spin structure is robust against scattering in a periodic step lattice with substantial disorder. A small but significant Rashba-type spin splitting could be observed also for quantum well states in ultrathin Pb films on Si(111), shedding more light on the mechanism of this effect [7]. And finally, spin polarization and spin texture could be measured for the first time on the surface of a topological insulator [8].

[1] S. LaShell et al., Phys. Rev. Lett. 77, 3419 (1996). [2] M. Hoesch et al., Phys. Rev. B 69, 241401 (2004). [3] M. Hoesch et al., J. Electron Spectrosc. Relat. Phenom. 124, 263 (2002). [4] F. Meier et al., Phys. Rev. B 77, 165431 (2008). [5] F. Meier et al., <http://arxiv.org/abs/1001.4927> [6] J. Lobo-Checa et al., Phys. Rev. Lett., in press (2010). [7] J. H. Dil et al., Phys. Rev. Lett. 101, 266802 (2008). [8] D. Hsieh et al., Science 323, 919 (2009).

3PL3



Public Interest Lecture: 20:00 Tuesday July 13, 2010

University of British Columbia

Life Sciences Institute 2

Catching Electrons with Light?

Paul Corkum

Joint Attosecond Laboratory, University of Ottawa & National Research Council Ottawa, Canada

In this, the 50th anniversary of the first laser, we are experiencing a revolution in one of the most important aspects of laser technology – the ability to make short flashes of light. Currently, the world's shortest light pulses are measured in attoseconds (1/1,000,000,000,000,000,000 of a second) – short enough to freeze the motion of valence electrons in atoms and molecules. Only 10 years ago, such an idea would have seemed like science fiction. This year too saw the first laser with a short enough wavelength to resolve the structure of complex biological molecules.

In our laboratory -- the Joint Attosecond Science Laboratory (JASLab) -- we have "photographed" a molecule's electrons and the position of its atoms – the first frame in a molecular movie which we plan to produce.

It was a century and a half ago that the very first movies were made. Containing only about a half dozen frames, the plots were boring -- but the images they contained were striking. It has taken us 150 years to refine the technology and the script to reach "Survivor". Today we stand on the verge of making real reality shows -- quantum movies that film chemical and biological processes as they occur. These films will give us unprecedented insight into the molecular world.



Paul Corkum (OC, FRS, FRSC) received his Ph.D. from Lehigh University, Bethlehem, Pa. In 1973 he joined the research staff of the National Research Council (NRC) of Canada. At NRC he concentrated first on laser technologies and then on using intense laser pulses to study and control matter. Paul is best known for introducing many of the concepts of how intense light pulses interact with atoms and molecules and then confirming them experimentally. He was the first to show how to make and measure attosecond pulses and how this new technology could be used to image atomic scale matter. Paul holds the Canada Research Chair of Attosecond Photonics at the University of Ottawa and serves as director of the Joint Attosecond Science Laboratory (JASLab). He is a member of the Royal Societies of London and of Canada, an Officer of the Order of Canada, and a member of the US National Academy of Science. Among his awards are the Canadian Association of Physicists' Gold Medal for Lifetime Achievement in Physics (1996), the Royal Society of Canada's Tory award (2003), the Optical Society's Charles H. Townes award (2005), the IEEE's Quantum Electronics Award (2005), the American Physical Societies' Schawlow prize (2006), the NSERC Polanyi prize (2008) and the American Chemical Societies Zewail Prize (2009). In 2009 he received NSERC's Herzberg Award, Canada's Highest Scientific Prize.

Poster Session 3P

3P - Tuesday, July 13, 14:00-16:00

*[Setup by 10:40 on Tuesday, July 13,
take down by 18:00 on Tuesday, July 13]*

The Poster Sessions take place in the East and West Atria of the Life Sciences Institute. The conference will not be responsible for posters that are left up after the above take down times.

3P Session Topic Breakdown

SURFACES & INTERFACES

OTHER

CORRELATED ELECTRON SYSTEMS

LOW DIMENSIONAL SYSTEMS

MAGNETISM

APPLICATIONS OF 3RD GENERATION LIGHT SOURCES

ATOMIC, MOLECULAR, OPTICS – EXPERIMENTAL

LIQUIDS & HIGH PRESSURE

SURFACES & INTERFACES

- 3P001 **Dengsung Lin**
Oscillatory electronic reconstruction at a buried ionic-covalent interface driven by surface reactions
- 3P002 **Evelina Domashevskaya**
Atomic and electronic structure peculiarities of the p-type porous silicon surface layers
- 3P003 **Evelina Domashevskaya**
Si L_{2,3} XANES and XPS investigations of 3d-metal/porous silicon nanostructures
- 3P004 **Daniil Karnaushenko**
Photoemission studies on the formation of top metallic contacts to organic films.
- 3P005 **Bonnie Leung**
Soft X-ray spectromicroscopy of protein interactions with model biomaterials
- 3P006 **Maria Luiza Rocco**
Photoabsorption and desorption studies on thiophene-based polymers following S K-shell excitation
- 3P007 **Xiulan Duan**
XPS studies of ZGSC nano-glass-ceramic materials
- 3P008 **Yuichi Haruyama**
Electronic structure of fluorinated diamond-like carbon thin films as a function of annealing temperature using photoelectron spectroscopy
- 3P009 **Bronislaw Orlowski**
High energy photoemission from buried layer of nanostructure
- 3P010 **Hiroshi Kumigashira**
Depth profiling for spin tunnelling junctions using hard-X-ray and soft-X-ray photoemission spectroscopy
- 3P011 **Lukasz Plucinski**
The surface electronic structure of ferromagnetic Fe(001) layers grown on W(001)
- 3P012 **Jian Jiang**
Temperature-dependent high-resolution angle-resolved photoemission study of the surface state in Al(100)
- 3P013 **Mao Ye**
Dirac electrons on the surface of topological insulators studied by angular resolved photoemission spectroscopy and scanning tunnelling microscopy
- 3P014 **Yao-Jane Hsu**
Modifying the cobalt surface by depositing a strong electron acceptor
- 3P015 **Yoshiyuki Ohtsubo**
Spin polarization of Shockley-type semiconductor surface state
- 3P016 **Kazutoshi Takahashi**
Electronic structures of the L-cysteine film on dental alloys
- 3P017 **Federica Bondino**
Ferromagnetic and ordered MnSi(111) epitaxial layers
- 3P018 **Stephen Urquhart**
X-ray photoemission electron microscopy of phase separated Langmuir-Blodgett thin films
- 3P019 **Takafumi Miyanaga**
Polarized XAFS study of Mg K-edge for MgB₂ on ZnO buffer lay

3P - TUESDAY, JULY 13, 14:00-16:00 *continued*

- 3P021 **Recardo Manzke**
The electronic band structure of β -Ga₂O₃ single crystals
- 3P022 **Kenta Kuroda**
Anisotropic Fermi surface of topological insulator Bi₂Se₃
- 3P023 **Galif Kutluk**
VUV light induced valence degeneration in Sm over-layer on HOPG
- 3P024 **Patrizia Borghetti**
Soft X-ray spectroscopy and DFT calculation studies on K-doped eumelanin in condensed phase
- 3P025 **Hirosuke Matsui**
Structure analysis of graphene grown on 4H-SiC(0001) surface by two-dimensional photoelectron diffraction
- 3P026 **Jean-Jacques Gallet**
Temperature programmed XPS (TPXPS) study of the desorption of ultra thin oxide films on silicon single crystals
- 3P027 **Tong Leung**
Hydrogen-bond mediated processes of glycine and diglycine on Si(111)7×7: A catch-and-release approach to surface functionalization
- 3P028 **Elena Filatova**
XPS and depth resolved SXES study of HfO₂/Si interlayers
- 3P029 **Giovanni Stefani**
Surface magnetic phase transitions revealed by Auger photoelectron coincidence spectroscopy
- 3P030 **Slavomir Nemsak**
Photoelectron spectroscopy study of an epitaxial ultra-thin alumina layer grown on Co(0001)

OTHER

- 3P031 **Victor Aristov**
Graphene synthesis on cubic SiC(001)/Si wafers
- 3P032 **Byron Freelon**
Pulsed Laser Deposition with in-situ synchrotron radiation-based high-resolution angle-resolved photoemission at MAESTRO

CORRELATED ELECTRON SYSTEMS

- 3P033 **Aleksey Murin**
Experimental and theoretical investigation of strongly correlated cerium-based systems
- 3P034 **Jean-Pascal Rueff**
Exploring the pressure - temperature phase diagram of strongly correlated materials: Application to critical valence fluctuations
- 3P035 **Jun Okamoto**
Magnetic structure at each Co ion in La_{1.5}Ca_{0.5}CoO₄ studied by site-selective resonant X-ray scattering
- 3P036 **Atsushi Yamasaki**
Hard and soft X-ray photoemission spectroscopy of A₂V₈O₁₆ (A=K, Rb)
- 3P037 **Mario Okawa**
Valence fluctuation in the heavy fermion YbAlB₄ system studied by hard X-ray photoemission spectroscopy
- 3P038 **Satoshi Toyoda**
Thermal stability of TiN/HfSiON/SiON gate stack structure on Si substrate studied by photoemission spectroscopy with in-depth profile analysis
- 3P039 **Kohei Yoshimatsu**
In situ angle-resolved photoemission study on SrRuO₃ thin films
- 3P040 **Recardo Manzke**
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- 3P041 **Akito Kakizaki**
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ARPES study of heavy-fermion systems at the reduced dimensionality
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- 3P046 **Masashi Arita**
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- 3P058 **Karen Paz Bastos**
Spectroscopic detection of spin-polarized bands and mixed valence for Ti and Sc in $\text{GdSc}_{1-x}\text{Ti}_x\text{O}_3$ for $x = 0.18$ and 0.25
- 3P059 **Leonardo Miotti**
Spectroscopic detection of Ti and Sc Fano and defect state resonances in high-resolution $L_{2,3}$ resonant photoemission spectroscopy (RPES) measurements
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Study of charge/orbital state in layered perovskite manganite $\text{Nd}_{2-x}\text{Sr}_x\text{MnO}_4$ by resonant X-ray scattering
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- 3P062 **Michael Sing**
Photoemission of a doped Mott insulator: spectral weight transfer and absence of metallic state
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Temperature dependent quasiparticle renormalization in nickel

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- 3P067 **Jau-Wern Chiou**
Correlation between electronic structures and photocatalytic activities of nanocrystalline-(Au, Ag, and Pt) particles on the surface of ZnO nanorods
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Wavelet investigation of EXAFS data for thin films of Mn doped Si based diluted magnetic semiconductors
- 3P069 **Takafumi Habuchi**
High-resolution photoemission spectroscopy of one-dimensional Pt complex $[\text{Pt}_2(\text{MeCS}_2)_4]_2\text{ClO}_4$
- 3P070 **Matthew Ward**
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- 3P071 **Satoru Motonami**
Particular kind of dispersive structures of TlSe investigated by angle-resolved photoemission spectroscopy

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- 3P072 **J.-S. Kang**
Soft X-ray absorption spectroscopy study of Mo-rich $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ perovskite oxides ($0.5 \leq x \leq 1$)
- 3P073 **Tetsuro Ueno**
Magnetic anisotropy and interface magnetism of Fe and Pd/Fe ultra-thin films on Pd(001) investigated by X-ray magnetic circular dichroism spectroscopy

- 3P074 **Hafiz Rafique**
Comparison of the electronic structure of $\text{LnBaCo}_2\text{O}_{5+\delta}$ ($\text{Ln} = \text{Gd}, \text{Dy}, \text{Dy}_{1-x}\text{Tb}_x, \text{Ln-112}$) and $\text{LnBaCo}_4\text{O}_7$ ($\text{Ln} = \text{Yb}, \text{Ln-114}$) single-crystal surfaces using resonant photoemission
- 3P075 **Patrik Grychtol**
Coupled magnetic multilayer systems studied by resonant reflectivity in the XUV range
- 3P076 **Chhayabrita Biswas**
Change in electronic structure within martensitic phase of $\text{Ni}_{50}\text{Mn}_{38}\text{Sn}_{12}$
- 3P077 **Shibo Xi**
Extreme vacuum ultraviolet magnetic linear dichroism investigations at Ni M-edge of NiO thin film
- 3P078 **Pieter Glatzel**
Strong K-edge magnetic circular dichroism detected by resonant inelastic X-ray scattering
- 3P079 **Yuta Miyata**
Soft X-ray photoemission study on antiperovskite manganites $\text{Mn}_3\text{Cu}_{1-x}\text{Ga}_x\text{N}$ ($x = 0, 0.5$)
- 3P080 **Philippe Leininger**
Electronic structure, magnetic and dielectric properties of the spin-chain compound NaCu_2O_2
- 3P081 **Jun Miyawaki**
Out-of-plane nesting-induced spin spiral in ultrathin Fe/Cu(001) films revealed by SX-ARPES
- 3P082 **Jae-Young Kim**
A practical approach correcting the saturation effect in XAS and XMCD spectra
- 3P083 **Byeong-Gyu Park**
X-ray absorption spectroscopy and X-ray magnetic circular dichroism study on the valence state and the spin structure of spinel $\text{Co}_{3-x}\text{Mn}_x\text{O}_4$ thin films
- 3P084 **Enju Sakai**
X-ray magnetic circular dichroism study of room-temperature ferromagnetism in Fe-doped TiO_2
- 3P085 **Takumi Ohtsuki**
Evidence for Ti 3d carrier-induced ferromagnetism in anatase $\text{Co}:\text{TiO}_2$ thin films

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Nano-roughness in gold revealed from X-ray signature
- 3P087 **Kazuo Soda**
Soft X-ray photoemission study of thermoelectric alloys $\text{Fe}_{2-x-y}\text{Ir}_y\text{V}_{1+x}\text{Al}$ and $\text{Fe}_{2-x}\text{V}_{1+x-y}\text{Ti}_y\text{Al}$
- 3P088 **Lijia Liu**
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- 3P089 **Masaki Kobayashi**
Change of Co distribution accompanied with degradation in membrane electrolyte assembly with Pt-Co cathode catalysts for PEFC
- 3P090 **Hiroyuki Kato**
Application of fluorescence-yield XAS to the studies of organic thin-film devices: observation of hidden electronic states and its field effect
- 3P091 **Jean-Pascal Rueff**
Overview of the GALAXIES beamline at the SOLEIL synchrotron: inelastic X-ray scattering and hard X-ray photoemission spectroscopy.
- 3P092 **Adam Leontowich**
Zone plate based soft X-ray lithography
- 3P093 **Tom Regier**
Silicon drift detector applications in soft X-ray absorption spectroscopy
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Resonant photoemission and X-ray absorption of organic Europium complexes
- 3P095 **Robert Blyth**
Resonant Auger at the Cu L_3 -edge of Cu_3Au : implications for resonant inelastic X-ray scattering (RIXS) and core-hole decay dynamics

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- 3P096 **Ron Cavell**
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LIQUIDS & HIGH PRESSURE

- 3P097 **Aleksey Murin**
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- 3P098 **Koichi Matsuo**
Solution-structure analysis of saccharides by synchrotron-radiation vacuum-ultraviolet circular dichroism spectroscopy
- 3P100 **Jin-Ming Chen**
Pressure-induced electronic and structural transformations in multiferroic BiMnO_3 probed by lifetime-broadening-suppressed X-ray absorption spectroscopy and X-ray emission spectroscopy
- 3P101 **Mercedes Hannelore Rittmann-Frank**
Behaviour of sodium halide ions in microscopic interfaces of mixed solvents observed via X-ray absorption spectroscopy

3P001

Oscillatory electronic reconstruction at a buried ionic-covalent interface driven by surface reactions

CT Lou,¹ HD Li,¹ JY Chung,¹ DS Lin,¹ TC Chiang²¹Department of Physics, National Tsing Hua University, Hsinchu, Taiwan; ²Department of Physics, University of Illinois, Urbana, United States

Lattice-matched ionic NaCl films were grown layer by layer on covalent Ge(100) using cycles of two half reactions that involved the alternative adsorption of Cl and Na. The Ge 3d photoemission spectra obtained after full cycles of growth resembled that of clean Ge(100), but came to resemble that of the polar Cl-terminated surface after the subsequent half reaction of Cl adsorption. Concurrently, the Na and Cl core levels of the nanofilms shifted by ~1.7 eV between these two interface configurations. Our results demonstrate that reactions on the NaCl surface drive periodic electronic reconstructions at the NaCl-Ge interface.

3P002

Atomic and electronic structure peculiarities of the p-type porous silicon surface layers

EP Domashevskaya,¹ VA Terekhov,¹ SY Turishchev,¹ DA Khoviv,¹ EV Parinova,¹ VA Skryshevsky,² IV Gavrilchenko²¹Solid State Physics and Nanostructures Department, Voronezh State University, Voronezh, Russian Federation; ²T.G. Shevchenko Kiev National University, Kiev, Ukraine

Atomic and electronic structure investigations of the porous silicon (p-type substrates) were performed with the use of the X-ray Absorption Near Edge Structure (XANES) spectroscopy and the UltraSoft X-ray Emission Spectroscopy (USXES) techniques. With the use of worked in XANES spectra parameters the relative depth of the oxide nanolayer of the porous silicon was examined together with Si-O bonds distortion character in silicon-oxygen tetrahedrons. XANES data reveals considerable changes in silicon oxygen tetrahedron accompanied with Si-O bonds tension and increasing of the Si-O-Si angles up to values close to coesite. This layer we named as the strained SiO₂. USXES data confirms these results and shows considerable amorphization of the investigate samples surface layers of porous silicon together with their oxidation revealing at the same time suboxide SiO_x. After about a year exposure in ambient atmosphere the porous silicon surface oxide layer depth lying on the amorphous layer covering silicon nanocrystals is few times greater than single crystalline silicon plates natural surface oxide layer. This work is based upon research supported by the Federal Targeted Program "Scientific and Scientific-Educational Personnel of the Innovative Russia".

3P003

Si L_{2,3} XANES and XPS investigations of 3d-metal/porous silicon nanostructures

VM Kashkarov,¹ AS Lenshin,¹ SY Turishchev,¹ EP Domashevskaya¹¹Solid State Physics and Nanostructures Department, Voronezh State University, Voronezh, Russian Federation

Electron energy structure of conduction band and silicon charge states in nanocomposites with magnetic properties on the basis of porous silicon (por-Si) with the deposited and co-deposited iron and cobalt were investigated by XANES (X-ray Absorption Near-Edge Structure) and XPS (X-ray Photoelectron Spectroscopy) techniques. The effect of 3d-metal deposition on silicon-oxygen bonds in porous silicon was demonstrated in the work. Previously we have shown that under deposition of Fe on the surface of porous silicon an almost continuous layer of iron and silicon oxides is formed on the surface while cobalt mainly penetrated deep into the pores forming metal nanoparticles coated with Co₂O₃ near the pore tips. As a result of XANES and XPS investigations it was found that 3d-metal deposition promoted a distortion of silicon-oxygen tetrahedrons on the surface of porous silicon and enhances the contribution of the defect oxide SiO_x into the oxide layer as compared with the original porous silicon. During natural ageing in the atmosphere (180 days) silicon oxide layer appeared on the surface of the samples of pure porous silicon and nanocomposites with Fe and Co with a thickness of ~ 5 nm exceeding the natural oxide layer on single-crystalline silicon.

3P004

Photoemission studies on the formation of top metallic contacts to organic films

D Karnaushenko,¹ J Ivanco,² T Toader,³ P Schäfer,¹ S Pop,⁴ D Marchenko,⁵ A Firsov,⁵ W Braun,⁵ DRT Zahn¹¹Chemnitz University of Technology, Chemnitz, Germany; ²Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia; ³Ruhr-Universität, Werkstoffe und Nanoelektronik, Bochum, Germany; ⁴Department of Solid State Physics, Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania; ⁵Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Formation of top metal contacts on an organic film, represented by indium (In) and antimony (Sb) evaporated on top of copper-phthalocyanine (CuPc) thin films, were investigated. The chemical and electronic structure of such metal-organic interfaces were examined via inspection of core levels and valence-band evolutions during the incremental deposition of metals. A component shifted toward high binding energy in the In 4d spectrum and gap states - the latter emerging between the highest-occupied molecular orbital (HOMO) and the Fermi level - which were recently regarded as an evidence of a reaction between In and CuPc [1], are consistently interpreted in terms of the final-state effect of finite and inert indium nanoclusters exposed at the CuPc surface. In contrast to In, the Sb 4d core level revealed no shifted components. As antimony tends to form significantly larger clusters, we assume that the Sb clusters become bulk-like in the photoemission final state.

3P005

Soft X-ray spectromicroscopy of protein interactions with model biomaterialsBO Leung,¹ AP Hitchcock,¹ JL Brash,² A Scholl,³ A Doran³¹Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON, Canada; ²Biomedical Engineering, McMaster University, Hamilton, ON, Canada; ³Advanced Light Source, Berkeley, CA, United States

Upon implantation in biological tissue or first contact with blood, all materials are immediately coated with a layer of proteins. The details of this initial protein layer can strongly affect biocompatibility. Thus, characterization of biomaterial surfaces and their interaction with relevant proteins can help understand and improve biocompatibility. We use synchrotron based X-ray photoemission electron microscopy (X-PEEM) and scanning transmission X-ray microscopy (STXM) to study the spatial distribution of proteins adsorbed on chemically heterogeneous surfaces. Both techniques have a lateral spatial resolution below 40 nm, provide speciation and quantitation through spatially resolved near-edge X-ray absorption fine structure (NEXAFS) spectroscopy, and can be used to obtain quantitative maps of the adsorbed protein in relation to the topography and chemistry of the underlying substrate with high sensitivity. X-PEEM probes the top 10 nm of the sample whereas STXM integrates over the full sample thickness (40-100 nm) and can be applied to fully hydrated samples. Results from two recent studies will be presented. [1] The effect of pentaerythritol triacrylate (PETA) crosslinker on the biocompatibility of PEO was examined with respect to crosslinker concentration. It was found that PETA is a highly surface active molecule and easily segregates to the substrate-air interface. Above 5 wt% PETA, HSA adsorption to the PETA-PEO surface markedly increases and reduces the biocompatibility of PEO. [2] HSA adsorption to polystyrene-poly(methyl methacrylate) spun-cast films was examined by STXM in a fully hydrated wet cell. In the presence of water, HSA preferentially adsorbs to the discrete polar PMMA domains rather than the continuous PS domain, whereas the latter is favored under dried conditions.

3P006

Photoabsorption and desorption studies on thiophene-based polymers following S K-shell excitationJR Santa Rita,¹ G Araújo,¹ C Arantes,¹ LS Roman,² AJG Zarbin,² MLM Rocco¹¹Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil; ²Federal University of Paraná, Curitiba, PR, Brazil

Photon stimulated ion desorption (PSID) and NEXAFS studies have been performed on thiophene-based polymers at the Brazilian Synchrotron Light Source following sulphur K-shell photoexcitation. For poly(thiophene) (PT) and poly(3-methylthiophene) (P3MT) it was found that the S $1s \rightarrow \pi^*, \sigma^*$ (S-C) excitation produces S⁺ desorption efficiently. On the other hand, S²⁺ desorption is strongly enhanced at excitations to higher energy orbitals. These results are interpreted in terms of the Auger-stimulated ion desorption mechanism. To our knowledge it is the first observation of multiple charged ions in PSID studies of polymers. For poly(3-hexylthiophene) (P3HT) S⁺ desorption seems to be suppressed, which may be due to the hexyl side-chains. Nanocomposites thin films made of P3HT and MWNT were also investigated. Both PSID mass spectra show great similarity, desorption of the polymer fragments only, and shift in the direction of greater time of flights for the composite. The relative desorption ion yield curves reproduce the photoabsorption spectrum. These results are discussed in terms of the indirect XESD process.

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3P007

XPS studies of ZGSC nano-glass-ceramic materialsX Duan,¹ D Yuan¹¹Shandong university, Jinan, Shandong, China

The transparent Co-doped ZnO-Ga₂O₃-SiO₂ nano-glass-ceramic composites were obtained by the sol-gel method. The Zn (2p_{3/2}), Ga (2p_{3/2}) and O (1s) XPS spectra for the glass-ceramics heat-treated at 800-1000°C could be deconvoluted into two peaks corresponding to these elements in glass network and in nanocrystals, respectively. The result indicates that the material is composed of an amorphous silicate network that encloses ZnGa₂O₄ nanocrystalline particles. Increasing the heating temperature of the annealed sample resulted in the further growth of the nanocrystalline particles.

3P008

Electronic structure of the fluorinated diamond-like carbon thin films as a function of annealing temperature using photoelectron spectroscopy

Y Haruyama,¹ Y Kang,¹ M Okada,¹ S Matsui¹

¹LASTI, University of Hyogo, Hyogo, Japan

The study of fluorinated diamond-like carbon (F-DLC) thin films has attracted much attention for wide applications because of the films' interesting properties, such as low friction coefficient, anti-stickiness, and chemical inertness. In the field of nanoimprint lithography, the F-DLC films were used as an anti-sticking layer of nanoimprint mold, for example. However, it was pointed out that the thermal stability in the F-DLC films was changed, depending on the temperature [1]. In this study, surface properties of the F-DLC films as a function of temperature were investigated using the photoelectron spectroscopy. At room temperature, several peaks at ~294, ~292, ~290, ~288, and ~286 eV were observed in the photoelectron spectra of the C 1s core-level in the F-DLC films. These peaks at ~294, ~292, ~290, ~288, and ~286 eV were assigned to the CF₃, CF₂, CF, C-CF, and C-C components, respectively [2]. With increasing the temperature up to 400 °C, the clear change was not observed. With increasing the temperature at more than 500 °C, CF₃, CF₂, and CF components decreased. In addition, the relative intensity of the F 1s peak to the C 1s peak decreased markedly. After annealing at 700 °C, the C-C component was dominant. Based on these photoelectron spectroscopy results, the temperature effect on the chemical composition and components is discussed.

[1] M. Jiang and Z. Ning, Surf. Coatings Tech. **200**, 3682 [2006]. [2] F. Quaranta et al., Appl. Phys. Lett. **63**, 10 [1993].

3P009

High energy photoemission from buried layer of nanostructure

BA Orłowski,¹ JB Pelka,¹ P Dziawa,¹ K Gas,¹ BJ Kowalski,¹ S Mickiewicz,² S Thiess,³ W Drube³

¹Institute of Physics PAS, Warsaw, Poland; ²Semiconductor Physics Institute, Vilnius, Lithuania; ³HASYLAB am DESY, Hamburg, Germany

Tunable High Energy X-ray Photoemission Spectroscopy (THE-XPS) study of nanostructure with Pb_{0.95}Eu_{0.05}Te layer buried in CdTe are presented. The MBE grown layer [1] Pb_{0.95}Eu_{0.05}Te 6nm, was deposited on CdTe 45nm, and then covered by CdTe 22nm thick, {100} plane. The experiment was performed at wiggler beam line station BW2 of the HASYLAB, DESY, Doris III storage Ring. Double (Si{111}) crystal monochromator covering an energy range from 2.4 to 10keV and with total energy resolution power of 0,5 eV was used. The CdTe top layer (22nm) was sputtered down to 7nm. The energy hν= 3510eV was used to obtain spectra containing: valence band, Cd3d and 4d, Pb 4f and 5d, Eu 3d, measured for different angles of incident of hν radiation. The change of relative height of Pb5d to the height of Cd4d and Te4d peaks versus the angles of light incident were determined in the region of standing wave critical angle. The standing waves electric field distribution in the nanostructure sample CdTe/PbEuTe/CdTe have been calculated with a program based on Parrat algorithm implementing the Fresnel recursive approach [2]. Calculated results explain the measured structure.

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1. M. Szot, et al., Acta Phys. Pol. **114**, 1397 [2009].

2. L. G. Parratt, Phys Rev. **95** [1954] 359

3P010

Depth profiling for spin tunnelling junctions using hard X-ray and soft X-ray photoemission spectroscopy

H Kumigashira,^{1,2,3} M Minohara,¹ K Horiba,^{1,3,4} E Ikenaga,⁵ M Oshima^{1,3,4}

¹Department of Applied Chemistry, The University of Tokyo, Tokyo, Japan; ²PRESTO, Japan Science and Technology Agency, Saitama, Japan; ³Synchrotron Radiation Research Organization, The University of Tokyo, Tokyo, Japan; ⁴CREST, Japan Science and Technology Agency, Tokyo, Japan; ⁵Spring-8/JASRI, Hyogo, Japan

Heterojunctions based on perovskite oxides have heralded the possibility of creating new multifunctional properties in ways that would not have been possible by using single-phase bulk materials. In order to design the devices based on oxides, it is indispensable to determine their band diagram precisely, in particular the potential profile in depth. In this study, we have performed a photoemission spectroscopy (PES) to directly determine the potential distribution in depth for promising spin tunnelling junctions between (a) a half-metallic ferromagnet La_{0.6}Sr_{0.4}MnO₃ (LSMO) and a semiconductor Nb-doped SrTiO₃ [Nb:STO]. Using the synchrotron radiation light ranging from soft X-ray to hard X-ray, the probing depth of PES measurements can be changed from 0.1 nm to 10 nm. The tunability of probing depth enables us to obtain the potential profile in depletion layers formed at the interface. The precise depth profiling analysis of LSMO/Nb:STO interfaces reveals the existence of a certain thin depletion layer of 1–2 nm with an abrupt potential drop near the interface. These results imply that the narrowing of the depletion layer is caused by the polar discontinuity at the LSMO [polar] /Nb:STO [nonpolar] interfaces.

3P011

The surface electronic structure of ferromagnetic Fe(001) layers grown on W(001)

L Plucinski,¹ Y Zhao,² B Sinkovic,² E Vescovo,³ CM Schneider¹

¹Institut f. Festkörperforschung IFF-9, Forschungszentrum Jülich, Jülich, Germany; ²Department of Physics, University of Connecticut, Storrs, CT, United States; ³National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY, United States

A thorough investigation of the surface electronic structure of thin ferromagnetic Fe(100) layers, epitaxially grown on W(001) single crystal, has been conducted using spin- and angle-resolved photoemission combined with state-of-the-art density functional theory slab-computations [1][2]. The dispersion of the surface state emission close to the Fermi level has been assessed quantitatively. The experimental results are in a good agreement with the calculations. In particular the presence of a minority surface state with d_{xz+yz} character along the surface GX high-symmetry direction is unambiguously established. Additionally, the calculations predict the existence of an unoccupied surface state localized at GX. The presence of the related minority interface resonance near the Fermi edge and outside of the surface-Brillouin-zone center GX is believed to control the tunneling magneto-resistance in Fe/MgO/Fe(001) for very thin MgO spacers. Our results indirectly confirm these predictions. Furthermore Fe/W(001) system has recently become prominent due to its application in the newest exchange-interaction based spin-detectors [3].

[1] L. Plucinski, Yuan Zhao, C. M. Schneider, B. Sinkovic, and E. Vescovo, Phys. Rev. B 80, 184430 (2009).

[2] L. Plucinski, Y. Zhao, B. Sinkovic, and E. Vescovo, Phys. Rev. B 75, 214411 (pages 8) (2007).

[3] A. Winkelmann, D. Hartung, H. Engelhard, C.-T. Chiang, and J. Kirschner, Rev. Sci. Instrum. 79, 083303 (2008).

3P012

Temperature-dependent high-resolution angle-resolved photoemission study of the surface state in Al(100)

J Jiang,¹ K Shimada,² H Iwasawa,² H Hayashi,¹ D Hirayama,¹ T Habuchi,¹ H Namatame,² M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima city, Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima city, Hiroshima, Japan

Aluminum is the textbook example of a trivalent nearly-free electron metal, and it is a BCS superconductor. In this study, we did high-resolution ARPES experiment on the Al(100) surface state to clarify the temperature dependence of the band dispersion and the electron-phonon interaction on the quasi-particles near the Fermi level. ARPES experiments were performed on the linear undulator beamline of a compact electron-storage ring (HiSOR) at Hiroshima University. We have observed a parabolic band dispersion of the Al(100) surface state centered at the Γ point. We found that the band bottom energy and the Fermi wavevector did not depend on temperature up to 300 K, which is different from the Shockley state in the noble metals [1]. At 50 K, we could observe a kink structure in the band dispersion which coincides well with the energy scale of the Debye temperature of Al. We have evaluated the coupling parameter of the electron-phonon interaction $\lambda_{el-ph} = 0.54$ at 50 K. We also found that the magnitude of the kink decreases above 50 K, indicating a decay of the quasi-particle state on heating.

[1] R. Paniago et al., Surf. Sci. 336, 113 (1995).

3P013

Dirac electrons on the surface of topological insulators studied by angular resolved photoemission spectroscopy and scanning tunneling microscopy

M Ye,¹ K Kuroda,¹ S Kim,¹ A Kimura,¹ K Miyamoto,² M Arita,² M Nakatake,² T Okuda,² K Shimada,² Y Ueda,³ M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³Kure National College of Technology, Kure, Japan

A novel class of quantum materials, called topological insulators (TI), which exhibits nontrivial surface states in a spin-orbit induced bulk energy gap, has invoked intensive interests both in the theoretical and experimental fields. An odd number of the surface states in this class of materials, such as Bi_2Sb , Bi_2Te_3 , and Bi_2Se_3 , promises the robust protection of the spin polarized surface states from the scattering by weak perturbation due to the time-reversal (TR) symmetry, which will essentially benefit the development of the novel quantum devices. Among the already discovered TI materials, Bi_2Se_3 , one of the "2nd-Generation TIs", shows the most promising properties, owing to the largest bulk energy gap with the simplest surface state totally exposed in the middle of it. In our present research, we have experimentally investigated the quasi-particle interference (QPI) on TIs against several kinds of surface and near-surface perturbations by means of scanning tunneling microscopy/spectroscopy (STM/STS), and angular-resolved photoemission spectroscopy (ARPES), in order to have a better understanding on the topologically protected surface states of TIs.

3P014

Modifying the cobalt surface by depositing a strong electron acceptorYJ Hsu,^{1,3} YL Lai,¹ YC Lin,¹ HT Chang,^{1,2} YJ Hung,^{1,2} YL Chan,¹ CH Wang,^{1,2} CH Lee,² DH Wei¹¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan; ³Institute of Electro-Optical Science and Engineering, National Cheng Kung University, Tainan, Taiwan

Organic spintronics has received increasing attention owing to its ability to integrate the emerging fields of organic semiconductor electronics and spin electronics. Exploiting the electronic and spin degree of freedom to carry information encoded with spin state and interact with magnetic materials motivates new functional electronic devices. For improving the electrical properties of the organic spintronics, the electrodes have to be energetically compatible with the organic semiconductors to form an ohmic contact for efficient charge injection. 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane [F4-TCNQ] with strong electron accepting character is utilized to modify the interface between the ferromagnetic cobalt and the organic layer, pentacene. The interface properties were studied by surface techniques like Synchrotron Photoemission Spectroscopy (PES), and Ultra-violet Photoemission Spectroscopy (UPS). Our UPS results reveal the deposition of F4-TCNQ can increase surface work function caused by surface dipole and decrease the hole-injection barrier for improving the device performance. The XPS spectra reveal direct evidence for a charge transfer-type interaction of F4-TCNQ with cobalt.

3P015

Spin polarization of Shockley-type semiconductor surface stateY Ohtsubo,^{1,2} K Yajji,^{1,2} S Hatta,^{1,2} H Okuyama,¹ K Miyamoto,³ T Okuda,³ A Kimura,⁴ H Namatame,³ M Taniguchi,^{3,4} T Aruga^{1,2}¹Department of Chemistry, Graduate School of Science, Kyoto, Japan; ²JST CREST, Saitama, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ⁴Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan

Much attention has been paid to the spin polarization of surface states because of the possibility of applications to spintronics. Recently, the spin polarization was observed on semiconductor substrates, such as Si and Ge, covered with heavy element [1, 2]. These spin-polarized states are localized at heavy atoms and hence experience strong spin-orbit interaction. On the other hand, the spin polarization of two-dimensional states in semiconductor subsurface layers has never been addressed yet. We have found a Shockley type surface-state band on Bi/Ge(111)-($\sqrt{3} \times \sqrt{3}$)R30°. We have characterized the band by spin- and angle-resolved photoelectron spectroscopy (SARPES). To provide insight into the electronic structure, a density-functional-theory (DFT) calculation based on the atomic structure determined by dynamical low-energy electron diffraction (LEED) analysis [3] is performed. This band is spread over several subsurface layers and is spin polarized due to the Rashba effect [4]. This result suggests that the contribution of heavy element is not always required for the surface-state spin polarization.

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3P016

Electronic structures of the L-cysteine film on dental alloysK Ogawa,¹ T Tsujibayashi,² K Takahashi,¹ J Azuma,¹ K Kakimoto,³ M Kamada¹¹Synchrotron Light Application Center, Saga University, Saga, Japan; ²Department of Physics, Osaka Dental University, Osaka, Japan;³Department of Geriatric Dentistry, Osaka Dental University, Osaka, Japan

Metal-organic interfaces have been attracting continuous attention in many fields including basic biosciences. The surface of dental alloys could be one of such interfaces since they are used in a circumstance full of organic compounds such as proteins and bacteria. In this work, electronic structures of Au-dominant dental alloys, which have Ag and Cu besides Au in different ratios, and L-cysteine on the surfaces have been studied by photoelectron spectroscopy with synchrotron radiation. It was found that the density of states in the dental alloys originate from gold and copper as constituents, and the Cu-3d states contribute dominantly to the occupied states near the Fermi level. It was also found that the electronic structure of the L-cysteine thin film on the dental alloys is different from that of the L-cysteine thick film. The results indicate the formation of the orbital bonding between Cu-3d and S-3sp states in the thin film.

3P017

Ferromagnetic and ordered MnSi(111) epitaxial layersF Bondino,¹ E Magnano,¹ C Cepek,¹ MC Mozzati,² E Carleschi,³ F Parmigiani³¹IOM CNR, Laboratorio TASC, Basovizza, Trieste, Italy; ²CNISM and Dipartimento di Fisica "A. Volta", Università di Pavia, Pavia, Italy;³Dipartimento di Fisica, Università degli Studi di Trieste, Trieste, Italy

The possibility of growing layers on semiconductors which are ferromagnetic at room temperature is of paramount importance for nonvolatile memories and spintronic devices based on the injection of spin-polarized current from a ferromagnetic metal into a semiconductor. In this perspective, MnSi films grown on Si substrate represent an interesting case study. Prompted by recent density-functional-theory calculations [1], predicting a ferromagnetic metallic ground state with a high degree of spin polarization at the Fermi level for MnSi films on Si (111), we have grown the epitaxial films in-situ and investigated their electronic and magnetic properties. The investigation has been performed using several techniques including SQUID magnetization measurements, low-energy diffraction (LEED), photoemission spectroscopy (PES), resonant photoemission spectroscopy (ResPES) and X-ray absorption spectroscopy (XAS). Our study provides clear proofs that these MnSi films have the same magnetic [3] and electronic [2] properties of bulk MnSi compound, so closing a long-standing question. Remarkably, the temperature dependence of the magnetization for the in-situ grown film and the MnSi single crystal are exactly the same, with the ferromagnetic state taking place below 50 K and with the maximum in the zero-field-cooled curve around 29 K when a low magnetic field (about 100 G) is applied. Furthermore, our measurements show the presence of a room-temperature ferromagnetic transition consistent with the ferromagnetic ground state predicted for Mn atoms with reduced coordination near surfaces and interfaces of silicon by recent calculations [1].

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[2] E. Carleschi et al. Surf. Sci. 601, 4066 (2007)

[3] E. Magnano et al. Appl. Phys. Lett., 96, 152503 (2010)

3P018

X-ray photoemission electron microscopy of phase separated Langmuir-Blodgett thin filmsSL Christensen,¹ SE Qaqish,¹ UD Lanke,^{1,2} MF Paige,¹ SG Urquhart¹¹Chemistry, University of Saskatchewan, Saskatoon, SK, Canada; ²Canadian Light Source, University of Saskatchewan, Saskatoon, SK, Canada

The structure and composition of phase-separated Langmuir-Blodgett (LB) monolayer films were characterized by X-ray photoelectron emission microscopy (X-PEEM) and atomic force microscopy (AFM). X-PEEM provides composition information with high lateral spatial resolution through the chemical sensitivity of NEXAFS spectroscopy, allowing us to perform chemical mapping of phase-separated domains in simple and complex mixed LB films. Model studies on simple mixed LB films (such as arachidic acid, C₁₉H₃₉COOH and perfluorotetradecanoic acid, C₁₃F₂₇COOH)[1] provide a basis for studies of mixed LB films with complex morphologies (such as palmitic acid, C₁₅H₃₁COOH, and perfluorooctadecanoic acid, C₁₇F₃₅COOH mixed LB films).[2] The use of energy filtered X-PEEM provides an energy resolved secondary electron emission microscopy (SEEM) mode, that provides a sensitive yet indirect structural and electronic sensitivity.

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3P019

Polarized XAFS study of Mg K-edge for MgB₂ on ZnO buffer layerI Miyanaga,¹ T Kanno,¹ Y Fujine,² M Yoshizawa²¹Department of Advanced Physics, Hirosaki University, Hirosaki, Japan; ²Faculty of Engineering, Iwate University, Morioka, Japan

Polarization dependent Mg K-edge XAFS study was carried out for MgB₂ films epitaxially deposited by MBE method on ZnO buffer layer. 50 and 150 nm MgB₂ films were deposited on the O-plane side of the ZnO single crystal. The investigation for O-plane side of ZnO is interesting because that the local structure of MgB₂ should be affected by Mg-O interaction on the ZnO. The Mg K-edge XAFS spectra were measured from the BL11A at Photon Factory of KEK. We obtained the following results: [1] Parallel to c-axis: Both of the interatomic distances of 1NN (1st nearest neighbor) Mg-B [2.487Å] and 3NN Mg-Mg [3.557Å] for 50 nm MgB₂ are shorter than that for 150 nm MgB₂ [2.506Å for Mg-B and 3.568Å for 3NN Mg-Mg]. [2] Perpendicular to c-axis: Both of the interatomic distances of 1NN Mg-B [2.521Å] and 2NN Mg-Mg [3.158Å] for 50 nm MgB₂ are longer than that for 150 nm MgB₂ [2.513Å for Mg-B and 3.151Å for 2NN Mg-Mg]. These results indicate that the structure of 50 nm MgB₂ film was expanded in the a-b plane and compressed to the c-axis, but that of 150 nm MgB₂ was relaxed apart from the ZnO surface and should be close to the MgB₂ crystalline. The fitting quality for 50 nm film as MgB₂ model is worse than that for 150 nm. This suggests that the reactive region by Mg and O atoms may exist between MgB₂ film and ZnO buffer layer.

3P021

The electronic band structure of β -Ga₂O₃ single crystals

M Mohamed,¹ C Janowitz,¹ Z Galazka,² R Uecker,² R Fornari,² R Manzke¹¹Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany; ²Leibniz-Institut für Kristallzüchtung, Berlin, Germany

β -Ga₂O₃ has the widest energy gap of the transparent conducting oxides (TCO). The interest in its electronic properties has recently increased because of its applications in various optoelectronic devices, semiconducting lasers, and ultrasensible gas detecting devices. In contrast, informations on the electronic structure of β -Ga₂O₃ are very scarce. Here we present the experimental valence band structure of β -Ga₂O₃ single crystals determined by high-resolution angle-resolved photoelectron spectroscopy (ARPES) utilizing HeI and synchrotron radiation. The high quality β -Ga₂O₃ single crystals were grown by using the Czochralski method and the {100} cleavage plane was characterized by several surface techniques, e.g. LEED and STM. It was found that the ARPES spectra along the parallel directions of the Brillouin zone show many very intensive peaks especially near the top of the valence band. However, the bands do not show much dispersion at 21.2 eV photon energy (HeI). On the other hand, with synchrotron radiation we were able to probe the direction normal to the surface and to determine with respect to \underline{k} perpendicular the Γ point at 30.0 eV. Here one observes distinct dispersion of the valence bands along all high-symmetric directions of the Brillouin zone. Furthermore, the valence band maximum and the band gap value of β -Ga₂O₃ could now be determined. The experimental valence band structure along the major symmetry lines will be discussed and compared with the theoretical results.

3P022

Anisotropic Fermi surface of topological insulator Bi₂Se₃

K Kuroda,¹ M Arita,² K Miyamoto,² M Ye,¹ A Kimura,¹ EE Krasovskii,^{3,4} EV Chulkov,^{3,4} J Jiang,¹ H Iwasawa,² T Okuda,² K Shimada,² Y Ueda,⁵ H Namatame,² M Taniguchi^{1,2}¹Graduated School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³Departamento de Física de Materiales, Facultad de Ciencias Químicas, San Sebastián, Spain; ⁴Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain; ⁵Kure National College of Technology, Kure, Japan

The three-dimensional topological insulator attracts a lot of attention in condensed matter physics. This new quantum phase of matter possesses a spin-helical surface state in the bulk-band gap, which can be distinguished from a conventional band insulator. This surface state is topologically protected, which restrains surface electron from backscattering induced by non-magnetic impurities and defects. However, recent some experiments of Bi₂Te₃ [1] have shown that there appears a quasi-particle interference pattern caused by hexagonal warping (HW) effect [2]. Up to now, it has been observed only in the case of Bi₂Te₃ that there is the hexagonally deformed Fermi surface (FS). Here, we present the first observation of the hexagonal deformation of FS in Bi₂Se₃, which has been believed to have an ideal Dirac cone so far, by means of angle-resolved photoemission spectroscopy. The photoemission spectra were taken linearly polarized light in which the electric field vector directed parallel and perpendicular to a mirror plane (p and s polarization). From the mapping of constant energy contours, it has been revealed that its shape evolves from a circle to a hexagon in going from the Dirac point towards the Fermi energy. The observed HW in the FS of Bi₂Se₃ is reproduced by the first principles calculation. [1] T. Zhang *et al.*, Phys. Rev. Lett. **103**, 266803 (2009). [2] Liang Fu, Phys. Rev. Lett. **103**, 266801 (2009).

3P023

VUV light induced valence degeneration in Sm over-layer on HOPG

G Kutluk,¹ M Nakatake,¹ H Sumida,² C Hong,¹ H Namatame,¹ M Taniguchi¹¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-hiroshimashi, Hiroshima, Japan; ²Technical research center, Mazda Motor Corporation, Aki-gun, Hiroshima, Japan

Samarium may be of particular interest from a fundamental point of view in physics of electronic structure since two different isoenergetic states may coexist: the free atomic Sm is divalent 4f⁶(sd)², but due to the gain in cohesive energy the bulk of metallic Sm is in a trivalent 4f⁵(sd)³. However, for the less coordinated Sm atoms in the surface layer the gain in the cohesive energy is smaller, and therefore the Sm atoms in the surface layer turn out to be divalent. Thus, the Sm coverage dependence of valence state has been one of the active subjects in the photoemission spectroscopy (PES) for the various systems consisting of the Sm over-layer over the past two decades. Nevertheless, the valence degeneration feature of Sm has been not completely understood [1]. On the other hands, we found clear time dependence of the degeneration of the Sm divalent state on VUV light-irradiation at $h\nu = 134$ eV with low coverage Sm over-layer on HOPG (highly oriented pyrolytic graphite) in recent work [2]. In this paper, we report the photon energy dependence of the photo-induced valence degeneration in detail by utilizing PES (UPS, XPS). We suggest that the effect of the VUV irradiation on the Sm valence state variation must be considered for a quantitative evaluation of valence state based on the UPS. The experiment was carried out using the BL7 of a compact electron-storage ring (HiSOR) at the Synchrotron Radiation Center, Hiroshima University. [1] M. Juel, B. T. Samuelsen, M. Kildemo, S. Raaen, Surf. Sci. 2006; 600, 1155, and references therein. [2] G. Kutluk, M. Nakatake, H. Sumida, H. Namatame, M. Taniguchi, Surf. Inter. Anal, in press.

3P024

Soft X-ray spectroscopy and DFT calculation studies on K-doped eumelanin in condensed phase

P Borghetti,¹ A Goldoni,² C Castellarin-Cudia,² L Floreano,³ A Cossaro,³ A Verdini,³ R Gebauer,⁴ P Ghosh,⁴ L Sangaletti¹

¹Università Cattolica, Brescia, Italy; ²Sincrotrone Elettra, Basovizza, Trieste, Italy; ³Laboratorio TASC, Basovizza, Trieste, Italy; ⁴The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy

Eumelanin is a ubiquitous biological pigment, with an intriguing combination of optical and electronic properties that have drawn the attention of materials physicists. The high affinity of natural eumelanin for metal ions opens up the perspective of controlling the functional properties by suitable doping. However, this possibility has not been thoroughly explored yet, mainly due to the practical difficulty in processing suitable eumelanin samples for chemical and physical analysis. In the present study, the effects of potassium on the electronic and morphological properties of eumelanin thin films deposited onto several conducting substrates is investigated by atomic force microscopy (AFM) and soft-X ray spectroscopies (XPS, NEXAFS, RESPES). In addition, experimental data are interpreted on the basis of density functional calculations for the isolated tetramers participating to the eumelanin macromolecule. AFM measurements provide evidences that K-doping promotes the self-assembly of spherical granules with lateral dimension of 50-200 nm, regardless the substrate and the deposition technique employed. Besides, a clear interaction of potassium atoms with nitrogen atoms in the molecule is attested. Finally, it is shown that K-doping also affects the low-lying states in the valence band, where a transfer of spectral weight across the HOMO-LUMO gap is observed, disclosing possible applications of this multi-functional biomacromolecule.

3P025

Structure analysis of graphene grown on 4H-SiC(0001) surface by two-dimensional photoelectron diffraction

H Matsui,¹ F Matsui,¹ N Nishikayama,¹ M Hashimoto,¹ K Goto,¹ N Maejima,¹ K Tanaka,¹ T Matsushita,² Y Kato,² T Okamoto,³ A N. Hattori,³ Y Sano,³ K Yamauchi,³ H Daimon¹

¹NAIST, Ikoma, Nara, Japan; ²JASRI/SPring-8, Sayo, Hyogo, Japan; ³Osaka University, Suita, Osaka, Japan

Graphene grown on SiC surface is expected to be the material for new generation devices. Its electronic property is strongly dependent on the structures of substrate and interface as well as the film thickness of graphene layer. Two-dimensional photoelectron diffraction (2D-PED) is a surface-sensitive and element-specific local atomic structure analysis method. We analyzed the structure of graphene on 4H-SiC(0001) surface at the various growth stages by 2D-PED using a display-type analyzer (DIANA) installed at circularly-polarized soft X-ray beamline BL25SU, SPring-8. Film thickness and lateral periodicity were characterized by angle-resolved XPS and RHEED. First, we examined the 2π -steradian C1s photoelectron intensity angular distribution (PIAD) of $6r3 \times 6r3$ surface prepared by annealing SiC at 800°C. Six forward focusing peaks (FFPs) were confirmed in addition to the SiC substrate diffraction pattern. Furthermore, we prepared monolayer and bilayer graphenes on SiC by controlled temperature annealing. We compared these 2π -steradian C1s PIADs with that of single crystalline graphite. Diffraction rings (DRs) due to the interference by the in-plane C-C bonds have been successfully separated from the interlayer diffraction patterns. Atomic distances are estimated from the circular dichroism of FFPs and DRs and also the radii of DRs. We report the surface structures of graphene on 4H-SiC(0001) based on the quantitative analysis of FFPs and DRs.

3P026

Temperature programmed XPS (TPXPS) study of the desorption of ultra thin oxide films on silicon single crystals

J J Gallet,¹ F Bournel,¹ F Rochet,¹ M Sully,² M El Kazzi,² F Sirotti²

¹LCPMR (UMR7614), Université P. et M. Curie, Paris 6, Paris, France; ²Synchrotron SOLEIL, Saint Aubin, France

The study of thermal decomposition of silicon oxide layer is essential for various reasons. For example the understanding of the thermal stability of gate oxides used in metal-oxide-semiconductor (MOS) is needed to make more reliable devices. In this study we use temperature programmed XPS to study the desorption kinetics of ultrathin oxide films formed on Si(111) substrates. The deoxidation reaction can be formally written as: $\text{SiO}_2 + \text{Si} \rightarrow 2 \text{SiO}_{\text{gas}}$. The Taylor-Weinberg approach is used to extract the activation energies E_a from the core-level kinetic data parameters (coverage q , temperature T and time t). With various velocities of temperature ramp, this approach allows to obtain activation energies and pre-exponential factor n depending of the coverage q which is not accessible by classical TPD experiment. Fast XPS acquisition necessary for such an experiment was performed on TEMPO beamline (SOLEIL, France) using the new three-dimension (x, y, t) delay line detector. The data acquisition time was reduced down to the ms/spectrum range. Various average temperature ramp velocities between ~ 2 K/s and ~ 100 K/s, were produced via Joule effect (voltage combs) while the photoemission spectra were recorded at zero bias. We observe that E_a increases with increasing coverage. For q comprised between 0.3 and 0.8, E_a ranges from 2.8 to 3.1 eV. Assuming a first order reaction, a pre-exponential factor n is determined ranging from 10^{13} s^{-1} ($q = 0.3$) to 10^{15} s^{-1} ($q = 0.8$), values expected on the basis of transition state theory.

3P027

Hydrogen-bond mediated processes of glycine and diglycine on Si(111)7×7: a catch-and-release approach to surface functionalization

L Zhang,¹ A Chatterjee,¹ T Leung¹¹WATLab & Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada

The growth of glycine and diglycine films by thermal evaporation on Si(111)7×7 at room temperature has been studied by X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). In contrast to the common carboxylic acids, glycine is found to adsorb on the 7×7 surface through dissociation of the N—H bond [instead of the O—H bond]. The presence of a transitional adlayer between the first adlayer and the zwitterionic multilayer is identified by its characteristic N 1s XPS features attributable to intermolecular N-to-HO hydrogen bond. An intramolecular proton transfer mechanism is proposed to account for the adsorption process through the amino group. We also demonstrate that the observed transitional adlayer can be used as a flexible platform to “catch-and-release” biomolecules with compatible H-bonding active sites in a controllable and reversible manner. Intricate evolution of the surface adsorption arrangement during the initial growth has also been monitored by STM. Early evidence of collective assembly of glycine into novel (dimeric) structures in the nanometer length scale could be found. These results are compared with the surface processes found for diglycine adsorption on the 7×7 surface.

3P028

XPS and depth resolved SXES study of HfO₂/Si interlayers

E Filatova,¹ A Sokolov,¹ A Ovchinnikov,¹ Y Savinov,¹ V Afanas'ev,² A Shulakov¹¹V.A. Fock Institute of Physics, St. Petersburg State University, St. Petersburg, Russian Federation; ²Department of Physics, University of Leuven, Leuven, Belgium

Nowadays HfO₂ is considered to be the most promising material for gate insulation in 45-nm technology node of metal-oxide-semiconductor (MOS) transistors and beyond. However, there is a problem arising from formation of an interlayer (IL) caused by oxidation of silicon during HfO₂ deposition: The formed SiO₂-like IL not only limits the gate stack downscaling but, also, affects electron and hole mobility in surface channels of Si MOS devices with HfO₂ insulation. The kinetics of the IL growth, its thickness and composition depend on large number of factors including the HfO₂ deposition method. A large number of incoming influences makes it difficult to predict *a priori* the IL properties. As a result, the formation of IL at the HfO₂/Si interface needs to be closely monitored. In this work we compare the HfO₂/Si structures with hafnia layers grown by atomic layer deposition (ALD) and metallo-organic chemical vapour deposition (MOCVD) techniques. We validated application of the X-ray emission spectroscopy with depth resolution (DRSXES) to HfO₂/Si interfaces by comparing its results to more conventional X-ray photoelectron spectroscopy (XPS) profiling technique. It is found that the atomic layer deposition of hafnia results in a thinner Si oxide interlayer than the metallo-organic chemical vapour deposition. It will be demonstrated the possibility of non-destructive chemical and structural analysis of layered samples using numerical simulation of the DRSXES data in the framework of the phenomenological Borovsky-Rydnik model adapted to a layered system. A good consistency between XPS and DRSXES results was found.

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3P029

Surface magnetic phase transitions revealed by Auger photoelectron coincidence spectroscopy

G Stefani,¹ F Offi,¹ A Ruocco,¹ F Da Pieve,¹ RA Bartynski,³ M Cini,⁴ R Gotter²¹Dipartimento di Fisica and CNISM, Università Roma Tre, Roma, Italy; ²IOM-CNR, Basovizza, Trieste, Italy; ³Department of Physics and Astronomy and Laboratory of Surface Modifications, Rutgers University, Piscataway, United States; ⁴INFN and Dipartimento di Fisica Università Tor Vergata, Roma, Italy

The origin of magnetic properties at the atomic level is a fundamental issue in physics and the investigation of how the electronic and magnetic structure of a solid changes when the magnetic order is established is of crucial interest in this respect. Nonetheless, spectroscopic probes that will directly sample the local magnetic moment are still missing. By using a moderate angular resolved detection, Auger Photoelectron Coincidence Spectroscopy (APECS) allows to selectively enhance or suppress the contribution from spin-symmetric and spin-antisymmetric final states. Hence, a new method for investigating the spin state of solid surfaces is provided. By means of this Dichroic Effect in APECS (DEAR-APECS) a sizable magnetic dichroism in the Auger lineshapes is achieved. DEAR-APECS has been used for investigating the electronic properties of a CoO thin film above and below the magnetic transition temperature T_N . In this way, we identify and assign, for the first time, well defined high-spin and low-spin structures in the otherwise featureless CoO Auger spectrum. Their temperature dependent intensity suggests a collapse of the surface magnetic properties at the atomic level, as well as at the macroscopic one, for temperatures just above T_N .

3P030

Photoelectron spectroscopy study of an epitaxial ultra-thin alumina layer grown on Co(0001)

S Nemsak,¹ M Yoshitake,¹ T Skala,² N Tsud³

¹National Institute for Materials Science, Advanced Electronic Materials Center, Tsukuba, Japan; ²Sincrotrone Trieste S.C.p.A, Materials Science Beamline, Basovizza-Trieste, Italy; ³Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

An epitaxial ultra-thin alumina layer was prepared on Co(0001) surface by simultaneous Al deposition and oxidation at elevated temperature. Oxide layer properties as well as the composition of the oxide-metal interface were examined by means of X-ray and ultra-violet photoelectron spectroscopy. Core-level photoelectron spectroscopy using Al-K_α and synchrotron-generated photons showed that the oxide-metal interface was formed by oxygen atoms. Angle-resolved X-ray spectroscopy measurements enabled depth profiling of the system and spectroscopically recognizable interface layer was found. P-type Schottky barrier height and work function was determined from valence band spectra. Low-energy electron diffraction revealed epitaxial parameters of the films and the relationship between the cobalt substrate and the oxide overlayer.

3P031

Graphene synthesis on cubic SiC(001)/Si wafers

YY Aristov,^{1,2} G Urbanik,¹ K Kummer,³ DV Vyalikh,³ OV Molodtsova,³ AB Preobrajenski,⁴ AA Zakharov,⁴ C Hess,¹ T Haenke,¹ B Buechner,¹ I Vobornik,⁵ J Fujii,⁵ G Panaccione,⁵ YA Ossipyan,² M Knuemper¹

¹IFW Dresden, Dresden, Germany; ²ISSP RAS, Chernogolovka, Russian Federation; ³ISSP TU Dresden, Dresden, Germany;

⁴MAX-lab Uni Lund, Lund, Sweden; ⁵TASC NL INFN-CNR, Trieste, Italy

The outstanding properties of graphene - single graphite layer, render it a top candidate for substituting silicon in future electronic devices. The so far exploited synthesis approaches, however, require conditions typically achieved in specialized laboratories, and result in graphene sheets whose electronic properties are often altered by interactions with substrate materials. The development of graphene-based technologies requires an economical fabrication method compatible with mass-production. Here we demonstrate for the first time the feasibility of graphene synthesis on, commercially available cubic SiC/Si substrates of > 300 mm in diameter, which result in graphene flakes electronically decoupled from the substrate [1]. After optimization of preparation procedure the proposed synthesis method can represent a further big step towards graphene-based electronic technologies.

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3P032

Pulsed laser deposition with in-situ synchrotron radiation-based high-resolution angle-resolved photoemission at MAESTRO

B Freelon,¹ I Furtado,^{1,2} A Orsini,³ P Medaglia,³ A Tebano,³ H Kohlstedt,⁴ A Bostwick,¹ Y Kim,¹ L Moreschini,¹ E Rotenberg,¹ J Pepper,¹ G Gaines,¹ R Ramesh,^{5,6} G Balestrino,³ Z Hussain¹

¹Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States; ²Applied Science and Technology Group, University of California Berkeley, Berkeley, CA, United States; ³INFN COHERENTIA and Dipartimento di Ingegneria Meccanica, Università di "Tor Vergata", Rome, Italy; ⁴Institut für Festkörperforschung and CNL, Forschungszentrum Jülich, Jülich, Germany; ⁵Department of Physics, University of California, Berkeley, Berkeley, CA, United States; ⁶Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

We report the integration of an ultra-high vacuum laser molecular beam epitaxy growth facility with a synchrotron-based high-resolution, angle-resolved photoemission (ARPES) 7.0.1.2 beamline at the MAESTRO facility of the Advanced Light Source. The laser-MBE deposition chamber is permanently attached to a series of ultra-high vacuum chambers for sample surface analysis, characterization and storage and ARPES experiments. In addition, to a suite of surface characterization tools, reflection high energy electron diffraction monitors the *in-situ* growth of transition metal oxide thin films that can be transferred under ultra-high vacuum to the high-resolution angle resolved photoemission spectroscopy endstation. The band mapping capability has an angular resolution < 0.1° based upon the GAMMADATA VG Scienta R-4000 ARPES spectrometer. The energy resolution of 25 meV is achieved for synchrotron beam energies from 80 to 1200 eV. The sample goniometer allows temperatures from 10K to 2200K. LaSrMnO₃ films were epitaxially deposited on strontium titanate (100) substrates. The system performance is demonstrated by bandstructural measurements of LaSrMnO₃/SrTiO₃[1 0 0] and SrTiO₃/SrTiO₃[1 0 0] grown. These films showed excellent transport and structural characteristics and yielded bandstructure that indicated the high quality of the materials.

3P033

Experimental and theoretical investigation of strongly correlated cerium-based systems

AV Murin,¹ IN Shabanova¹¹Physicotechnical Institute of the Ural Division of the Russian Academy of Sciences, Izhevsk, Russian Federation

The class of the compounds based on f-elements (Ce) attracts significant attention because of their unusual properties. These systems refer to the class of compounds with strong correlations. In the present work, the electronic structure and the regularities of the formation of the relaxed final state of the CeCu₆, CePd₃, CeSi₂ and CeF₃ systems were investigated by the X-ray photoelectron spectroscopy (XPS) method. The calculation of the total and partial density of states (DOS) was conducted by the ab-initio band structure calculation methods allowing to take into account the covalent character of the bond. The used calculation methods are single-electron methods and they do not take into account the strong correlation effects. However, the chosen approximation is adequate because it adequately reflects the shape of the valence bands obtained experimentally. The results of the calculations of the total DOS are in good agreement with the results of the XPS spectra of the valence bands of the systems under study. The difference in the electronic structure between ordinary Ce-based systems and the Ce-based systems (CeCu₆, CePd₃, CeSi₂) passing in the heavy-fermion state at low temperatures is the strong hybridization of the outer shell electrons of neighboring atoms of heavy-fermion systems including 4f states nearby Fermi level, which partially overlap with the external localized states. Thus, in strongly correlated Ce-based systems even in the non-heavy-fermion state, an unusually high interatomic interaction is observed. It explains why the breaking strength of components of machines and machinery improves by several orders of magnitude when a layer (tens of Å) from a strongly correlated Ce-based compound is applied on their surface.

3P034

Exploring the pressure - temperature phase diagram of strongly correlated materials: Application to critical valence fluctuations

JP Rueff^{1,2}¹Synchrotron SOLEIL, Gif sur Yvette, France; ²Laboratoire de Chimie Physique - Matière et Rayonnement, UPMC - CNRS, Paris, France

The remarkable properties of strongly correlated materials largely originate from the subtle coupling between the electronic, structural and spin degrees of freedom. The coupling strength may be effectively modified by applications of external parameters such as pressure, temperature or doping, triggering transitions in their physical properties. This calls for new ways of exploring the phase diagram of strongly correlated electrons from the point of view of the electronic properties. To that aim, inelastic X-ray scattering (IXS) has emerged as one of the most powerful methods [1]. Lately, we have investigated by IXS the phase diagram of several the f- and d-strongly correlated electrons systems under combined pressure-temperature conditions. We will here more specifically focus on recent results obtained in CeCu₂Si₂, the first discovered heavy fermion superconductor. Using high-resolution X-ray absorption spectroscopy at the Ce L₃ edge in the partial fluorescence yield mode - a technique derived from resonant IXS that provides spectra partly free from core-hole lifetime broadening -, and aided by full multiplet calculations, we have estimated for the first time the Ce valence in the vicinity of the superconducting phase under pressure at low temperature. The results provide strong hints for significant valence changes near the superconducting dome in CeCu₂Si₂ in remarkable agreement with the new pairing mechanism based on critical valence fluctuations proposed for f-electron materials.

[1] J.-P. Rueff et al., Rev. Mod. Phys. **82**, 847 (2010)

3P035

Magnetic structure at each Co ion in La_{1.5}Ca_{0.5}CoO₄ studied by site-selective resonant X-ray scattering

J Okamoto,¹ K Horigane,² H Nakao,¹ M Kubota,¹ K Amemiya,¹ Y Murakami¹¹IMSS, KEK, Tsukuba, Ibaraki, Japan; ²WPI-AIMR, Sendai, Miyagi, Japan

La_{2-x}Ca_xCoO₄ system has been controversial for its Co³⁺ spin states, which takes an important part in the peculiar deviation of magnetization via Ca concentration. Co²⁺ ion always takes high-spin (HS) states, but Co³⁺ ion takes various spin states, estimated from magnetization measurements; HS for x < 0.5 and intermediate-spin (IS) for x > 0.7. La_{2-x}Ca_xCoO₄ takes two kinds of magnetic structures below Neel temperature with scattering vector q = {1/2, 0, 1/2} and {1/2, 0, 1}. For x < 0.5 only {1/2, 0, 1/2} structure is observed, and for x > 0.5 only {1/2, 0, 1} structure is observed by neutron scattering. For x = 0.5 both {1/2, 0, 1/2} and {1/2, 0, 1} are observed. Therefore, it is important to reveal the difference of magnetic structures with q = {1/2, 0, 1/2} and {1/2, 0, 1} and their relationship with Co-site electronic structures. We have measured energy scan of scattering intensities with q = {1/2, 0, 1/2} and {1/2, 0, 1} of La_{1.5}Ca_{0.5}CoO₄ by resonant soft X-ray scattering at BL16A, KEK-PF, and compared them with XAS spectra and theoretical calculations to determine the electronic structures which take part in these magnetic structure and relationship with deviation of magnetization by Ca doping.

3P036

Hard and soft X-ray photoemission spectroscopy of $A_2V_8O_{16}$ ($A=K, Rb$)

A Yamasaki,¹ A Higashiya,² S Imada,³ A Sekiyama,⁴ H Fujiwara,⁴ J Yamaguchi,⁴ M Yabashi,⁵ K Tamasaku,⁵ T Ishikawa,⁶ T Muro,⁵ Y Kato,⁵ H Kobori,¹ A Sugimura,¹ M Isobe,⁷ Y Ueda,⁷ S Suga⁴

¹Faculty of Science and Engineering, Konan University, Kobe, Japan; ²Industrial Technology Center of Wakayama Prefecture, Wakayama, Japan; ³College of Science and Engineering, Ritsumeikan University, Kusatsu, Japan; ⁴Graduate School of Engineering Science, Osaka University, Osaka, Japan; ⁵JASRI/SPring-8, Sayo, Japan; ⁶RIKEN/SPring-8, Sayo, Japan; ⁷ISSP, University of Tokyo, Kashiwa, Japan

Recently, hollandite-type transition-metal oxides have attracted much attention due to their exotic behaviors. Among them, the vanadium oxide $A_2V_8O_{16}$ ($A=K, Rb$) shows the metal-insulator transition (MIT), the temperature of which depends on the cationic species. By changing the cationic species from potassium to rubidium, it was reported that the lattice volume and the MIT temperature increase. We report the bulk electronic structures of hollandite-type vanadium oxide $A_2V_8O_{16}$ ($A=K$ and Rb) studied by high-energy photoemission spectroscopy. The hard-x-ray and the soft-x-ray photoemission spectroscopy (HAXPES and SXPES) were performed at the beamline BL19LXU and BL27SU in SPring-8. The inelastic mean free path of photoelectrons in the HAXPES experiment for the valence band is about 10 times longer than the in-plane lattice constant of $K_2V_8O_{16}$, which provides high bulk sensitivity. We have observed the coherent quasi-particle peak in the metallic phase of $K_2V_8O_{16}$. In addition, the existence of the coherent component in the insulating phase is revealed as predicted by the dynamical mean field theory for VO_2 .

3P037

Valence fluctuation in the heavy fermion $YbAlB_4$ system studied by hard X-ray photoemission spectroscopy

M Okawa,¹ M Matsunami,² K Kuga,¹ K Ishizaka,³ R Eguchi,⁴ M Taguchi,⁵ A Chainani,⁵ Y Takata,⁵ M Yabashi,^{5,6} K Tamasaku,⁵ Y Nishino,⁷ T Ishikawa,^{5,6} N Horie,¹ S Nakatsuji,¹ S Shin^{1,5}

¹Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba, Japan; ²UVSOR Facility, Institute for Molecular Science, Okazaki, Aichi, Japan; ³Department of Applied Physics, University of Tokyo, Tokyo, Japan; ⁴Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan; ⁵RIKEN SPring-8 Center, Sayo, Hyogo, Japan; ⁶Japan Synchrotron Radiation Research Institute, Sayo, Hyogo, Japan; ⁷Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan

β - $YbAlB_4$ is the first Yb-based heavy fermion system to show superconductivity ($T_c = 80$ mK). This superconductivity is considered to appear around a quantum critical point (QCP) existing without external tunings (i.e., magnetic field, pressure, or chemical doping), so that we can investigate the electronic structures in the vicinity of the QCP using photoemission spectroscopy (PES). Here, we report the bulk-sensitive hard X-ray (7.94 keV) PES study on β - $YbAlB_4$ and its polymorph α - $YbAlB_4$ which is the Fermi liquid system, performed at beamline BL29XUL of SPring-8. In Yb 3d core level spectra, divalent and trivalent components of Yb were clearly found, which is the direct evidence for the intermediate valence state. The estimated Yb valences of ~ 2.7 - 2.8 indicate that the 4f electrons are well itinerant. The strong valence fluctuation occurring near the QCP in β - $YbAlB_4$ is unique in comparison with other Yb-based compounds. Our results may suggest an important role of the valence fluctuation in addition to the magnetic fluctuation in the quantum criticality and its relation to the superconductivity. Besides the above results, we report our recent study revealing the valence fluctuation remaining in the Fe-doping induced antiferromagnetic region in α - and β - $Yb(Al,Fe)B_4$.

3P038

Thermal stability of TiN/HfSiON/SiON gate stack structure on Si substrate studied by photoemission spectroscopy with in-depth profile analysis

S Toyoda,^{1,2,3} H Kamada,¹ H Kumigashira,^{1,3,5} M Oshima,^{1,2,3} K Iwamoto,⁴ T Sukegawa,⁴ Z Liu⁴

¹Department of Applied Chemistry, The University of Tokyo, Tokyo, Japan; ²Core Research for Evolutional Science and Technology, Japan Science and Technology Agency, Tokyo, Japan; ³Univ-of-Tokyo Synchrotron Radiation Research Organization, Tokyo, Japan; ⁴Semiconductor Technology Academic Research Center, Kanagawa, Japan; ⁵Precursory Research for Embryonic Science and Technology of Japan Science and Technology Agency, Tokyo, Japan

Metal gate electrodes/high permittivity (high-k) oxide films are widely studied to replace conventional poly-Si/SiO₂ systems for further downscaling of metal-oxide-semiconductor devices. Interfacial reactions during annealing processes for dopant activation are one of the most serious issues due to a degradation of electrical properties such as large leakage current and threshold voltage shift. Thus it is necessary to investigate the mechanism of interfacial reactions to control them. In this study, we have investigated thermal stability of TiN/HfSiON/Si gate stack structures by angular-dependent photoemission spectroscopy with in-depth profile analysis. 2-nm-thick HfSiON layers were deposited on clean p-type Si substrates by atomic layer deposition, followed by TiN deposition using RF reactive sputtering. Each sample was annealed at 850, 950 and 1050°C under nitrogen gas ambient. Photoemission measurements were then carried out at the undulator beamline BL-2C of the Photon Factory in KEK. Annealing temperature dependence of Si 2p core-level spectra shows monotonous growth of Si oxide component with increasing annealing temperature. We also found that a remarkable growth of Si-oxide components at the surface of the TiN metal gate electrode by in-depth profile analysis. These unusual Si-oxidation reactions can be attributed to the formation of Ti-silicide component at the TiN/HfSiON interface, which is observed at the as-grown stage after TiN deposition.

3P039

In situ angle-resolved photoemission study on SrRuO₃ thin filmsK Yoshimatsu,¹ H Kumigashira,^{1,2,3} A Fujimori,⁴ M Oshima^{1,3,5}¹Department of Applied Chemistry, The Univ. of Tokyo, Tokyo, Japan; ²PRESTO, Japan Science and Technology Agency, Saitama, Japan; ³SRRO, The Univ. of Tokyo, Tokyo, Japan;⁴Department of Physics, The Univ. of Tokyo, Tokyo, Japan; ⁵CREST, Japan Science and Technology Agency, Tokyo, Japan

Perovskite-type Ru oxides exhibit the unusual physical properties such as the superconductivity-metal-insulator transition in Ca_{2-x}Sr_xRuO₄ and the ferromagnetic-paramagnetic transition in Ca_{1-x}Sr_xRuO₃. In order to clarify the origin of these physical properties, it is essential to obtain the information on the band structures of these oxides, especially the Fermi surface (FS) topology. Angle-resolved photoemission spectroscopy (ARPES) is one of the best experimental ways to determine the band structures. However, there are few ARPES studies on Ca_{1-x}Sr_xRuO₃ owing to the absence of any cleavage surfaces, which is in sharp contrast to the intensive ARPES studies on layered Ca_{2-x}Sr_xRuO₄ having cleavable planes.

In this study, we have performed *in-situ* soft X-ray ARPES studies on well-ordered surfaces of single-crystal SrRuO₃ thin films grown by laser molecular beam epitaxy. We clearly observed the several band dispersions indicative of the clean and well-ordered surface of SrRuO₃ thin film. From the FS mapping, it is found that the FS of SrRuO₃ consists of electron pockets centered at the Γ point and hole pockets at the M point. The observed FS's are in good agreement with the prediction from the band structure calculations [1].

[1] G. Santi et al., J. Phys. Condens. Matter **9**, 9563 [1997].

3P040

Charge density wave transition of TiSe₂R Manzke,¹ M May,¹ C Janowitz¹¹Institute of Physics, Humboldt-University of Berlin, Berlin, Germany

The driving force of the charge density wave (CDW) phase of the transition metal dichalcogenide TiSe₂ in competition to other charge order mechanisms like superconductivity is still under intense discussion. One crucial question for a microscopic understanding of its origin and related models was that on the electrical character of the material, i.e. whether TiSe₂ is a semiconductor or a semimetal. By means of angle-resolved photoemission (ARPES) applying controlled band bending due to the adsorption of polar molecules onto the van der Waals-like surface, Rasch et al., [PRL 101, 237602 [2008]] undoubtedly identified TiSe₂ as a small-gap semiconductor. For the study of the CDW the adsorption experiments were extended to temperatures ranging from 10K to 300K. It reveals that additional population of the Ti 3d conduction band leads to a gradual suppression of the CDW phase. In addition, a weak increase or decrease of the gap by utilizing the ternary crystals TiSe_{2-x}S_x and TiSe_{2-x}Te_x, resp., reveals information on the optimal gap value. These results will be discussed with regard to the existing models.

3P041

Valence band structures of MSi(001) (M= Mn, Fe, Co) obtained by angle-resolved photoemission spectraA Kakizaki,¹ Y Takeichi,¹ A Nishide,¹ T Okuda,¹ F Komori,¹ K Nakatsuji,¹ J Yoshinobu,¹ I Matsuda,¹ A Harasawa,¹ H Kondoh,² F Bertran,³ P Le Ferve,³ A Taleb-Ibrahimi,³ H Yamagami⁴¹Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba, Japan; ²Department of Chemistry, Keio University, Yokohama, Kanagawa, Japan; ³SOLEIL / LURE, Gif-sur-Yvette, Cedex, France; ⁴Department of Physics, Kyoto Sangyo University, Kamigamo, Kyoto, Japan

We have measured high-resolution angle-resolved photoemission (ARPES) spectra of transition metal mono-silicide single crystals, MSi(001) (M= Mn, Fe, Co) and studied their electronic structures. The valence band structures of iso-structural MSi(001) obtained from ARPES spectra are basically consistent with those by theoretical calculation, except with the 30% smaller band width in FeSi(001) than that expected from the calculation due to the renormalization effect [1]. In FeSi(001), Fe 3d originated bands show a very small energy dispersion close to the Fermi level with an energy gap of 20 meV below it. In CoSi(001), the observed valence band structure well agrees with that of calculation and shows a dip structure at the binding energy of 0.5 eV with the width of about 100 meV, which corresponds to the energy gap in the valence bands. Our result resolves the controversial evidences, which have been provided for the arguments of the Kondo-insulator in FeSi [1] and the valence fluctuation in MnSi [2].

[1] M. Klein, D. Zur, D. Menzel, J. Schoenes, K. Doll, J. Röder and F. Reinert, Phys. Rev. Lett. **101**, 046406 [2008].

[2] K. Kura, K. Takano, Y. Takeichi, A. Harasawa, T. Okuda, I. Matsuda and A. Kakizaki, J. Phys. Soc. Jpn. **77**, 024709 [2008].

3P042

Energy and doping dependences of quasiparticle group velocity and coupling spectrum in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

H Anzai,¹ A Ino,¹ T Kamo,¹ T Fujita,¹ M Arita,² H Namatame,² M Taniguchi,^{1,2} A Fujimori,³ Z X Shen,⁴ M Ishikado,³ S Uchida³

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan;

³Department of Physics, University of Tokyo, Tokyo, Japan; ⁴Department of Applied Physics and SSRL, Stanford University, Stanford, CA, USA

Physical properties of solid are characterized by electron dynamics that relies on the interaction of electrons with collective excitations. Thus, understanding of the many-body effects in high-Tc cuprates may provide us a possible candidate of mediator that forms Cooper pair. Recently, strong mass renormalization has been observed in underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ [1]. However, its origin and relation to the mechanism of high-Tc superconductivity remain unclear. Here, we present the energy, doping and band dependence of quasiparticle group velocity and coupling spectrum, deduced from low-energy angle-resolved photoemission spectra of Bi2212. The experiments were performed at HISOR BL-9A in Hiroshima Synchrotron Radiation Center. The small nodal bilayer splitting has clearly been resolved for underdoped, optimally-doped and overdoped samples. Our result indicates that the mass enhancement in underdoped Bi2212 occurs at low energies almost independent on the bilayer-split bands, and that the energy of dominantly coupled excitations change from $|\omega| \sim 65$ meV to $|\omega| \sim 15$ meV with underdoping.

[1] I. M. Vishik *et al.*, arXiv:1002.2630.

3P043

ARPES study of heavy-fermion systems at the reduced dimensionality

SL Molodtsov,^{1,2} DV Vyaliikh,² S Danzenbaecher,² Y Kucherenko,^{2,3} C Laubschat,² C Krellner,⁴ C Geibel⁴

¹European XFEL GmbH, Hamburg, Germany; ²University of Technology, Dresden, Germany; ³Institute for Metal Physics, Kiev, Ukraine; ⁴MPI for Chemical Physics of Solids, Dresden, Germany

Electron-hybridization phenomena in Yb- and Eu-transition metal (TM) heavy-fermion compounds were probed by ultra-high resolution angle-resolved photoemission (ARPES) [1-4] and reveal strong momentum (\mathbf{k}) dependent splittings of the $4f$ emissions around the expected intersection points of the $4f$ final states with valence bands in the Brillouin zone. The obtained dispersion of the interacting $4f$ states is explained in terms of a simplified periodic Anderson model (PAM) by \mathbf{k} dependence of the electron hopping matrix element ruling out interpretation in terms of a single-impurity Anderson model (SIAM) for single-crystalline samples. The Yb(Eu) $4f$ -TM d hybridization strength in the surface region of these correlated materials can be varied by doping or deposition of metallic overlayers. Site-specific charge transfer from the dopants or adatoms leads to change of the energy overlap of the interacting states close to the Fermi energy. We show that the electron-correlation properties like heavy-fermion and Kondo behavior at the reduced dimensionality can be tuned and are rather different from the bulk material.

[1] D.V. Vyaliikh *et al.*, PRL 103 [2009] 137601

[2] S. Danzenbächer *et al.*, PRL 102 [2009] 026403

[3] D.V. Vyaliikh *et al.*, PRL 100 [2008] 056402

[4] S. Danzenbächer *et al.*, PRL 96 [2006] 106402

3P044

Strong spin-orbit coupling in Sr_2RuO_4 : what is the fate of spin-triplet superconductivity?

M Raichle,¹ C Veenstra,¹ D Fournier,¹ M Haverkort,² I Elfimov,¹ A Damascelli¹

¹PHAS, UBC, Vancouver, BC, Canada; ²Anderson, MPI-FKF, Stuttgart, BW, Germany

Recent local density approximation plus spin-orbit coupling (LDA+SOC) band structure calculations showed that SOC is essential in describing the Fermi surface (FS) of Sr_2RuO_4 [1]. Moreover these calculations predict an interesting spin-anisotropy in that compound, which shows that spin-singlet and spin-triplet states are mixed. We are performing a spin- and angular-resolved photo-emission spectroscopy (SARPES) experiment and we expect to verify this spin-anisotropy. These experiments might provide compelling evidence that pure spin-triplet p-wave superconductivity on the gamma sheet [2] is too simple a picture for Sr_2RuO_4 .

[1] M. W. Haverkort *et al.*, PRL 101, 026406 [2008],

[2] T. M. Rice and M. Sigrist, J. Phys.: Condens. Matter 7, L643 [1995].

3P045

Elusive electron-phonon coupling in quantitative spectral function analysisCN Veenstra,¹ GL Goodvin,¹ M Berciu,¹ A Damascelli¹¹Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada

Angle-resolved photoemission spectroscopy (ARPES) provides access to the electron-removal part of the momentum-resolved spectral function. This quantity is an extremely rich data source, as it depends on both the bare electronic dispersion as well as electronic correlations. Interpretation of ARPES data has often relied on two approaches - quasiparticle and self-energy methods. Quasiparticle methods focus on an observed dispersion relation and its renormalization compared to the bare band, often with an assumed link between coupling strength and these renormalizations through the so-called mass enhancement factor $(1+\lambda)$. This link, however, has been merely phenomenological and its general validity needs verification. Self-energy methods, where observed peak positions and widths are related to the real and imaginary parts of the self-energy of the correlations, often rely on assumptions about the form of the self-energy as well as bare electronic structure. With the new, highly accurate, momentum average approximation we simulate spectral functions for electron-phonon coupling and test both techniques for extracting information from ARPES data [1]. We show that the effective coupling parameters deduced from the renormalization of quasiparticle mass, velocity, and spectral weight are momentum dependent and, in general, distinct from the true microscopic coupling. We show that the non-linear relationship between these quantities could easily lead to a mis-estimation of the microscopic coupling by factors ranging anywhere from 2 to 10. We also find that, in the low-coupling regime, it is possible to extract self-energy through a self-consistent Kramers-Kronig bare-band fitting routine with minimal assumptions about the bare electronic structure, in cases where the self-energy is not strongly momentum dependent.

[1] C.N. Veenstra, G.L. Goodvin, M. Berciu, A. Damascelli, arXiv:1003.0141 [2010]

3P046

Angle-resolved photoemission study of a narrowgap semiconductor FeGa₃M Arita,¹ K Shimada,¹ H Namatame,¹ M Taniguchi,^{1,2} Y Hadano,³ T Takabatake³¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan;³Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima, Japan

FeGa₃ with a tetragonal structure is one of the iron-based narrowgap semiconductors that are expected as novel thermoelectric materials. A band-structure calculation predicted an indirect gap of 0.3 eV, and the valence-band maximum (VBM) at the A point.[1] We have performed angle-resolved photoemission spectroscopy (ARPES) of FeGa₃, in order to experimentally clarify the band structure. ARPES measurements were carried out using photon energy of $h\nu = 21$ eV on the helical undulator beamline of HiSOR. The energy-band dispersions around the A point were examined using cleaved single crystalline samples with the {111} surface. Two flat bands derived from the Fe 3d state were observed at $E_b = 0.5$ and 1 eV. We also observed dispersive bands which can be attributed to the Ga 4s and 4p states. Between the shallower flat band and E_b , a hole-like dispersive band was observed in agreement with the band calculation. We found no quasi-particle peak at VBM nor narrowing of the band width. Therefore FeGa₃ is not a strongly correlated electron system like FeSi.[2] Our observations are consistent with conventional semiconducting behaviors found by the electrical resistivity and specific heat coefficient measurements.[3]

[1] Y. Imai et al., Intermetallics 14[2006] 722. [2] V. Jaccarino et al., Phys. Rev. 160[1967] 476.

[3] Y. Hadano et al., J. Phys. Soc. Jpn. 78[2009] 013702.

3P047

Study of electronic states near Fermi level of quasi-one-dimensional vanadium oxide NaV₂O₅ by angle-resolved photoemission spectroscopy at low-excitation energyA Higashiya,^{1,2} A Irizawa,² M Tsunekawa,² A Yamasaki,² A Sekiyama,² S Imada,² S Suga,² M Arita,³ Y Takeda,^{3,4} H Namatame,³ M Taniguchi,³ M Isobe,⁵ Y Ueda⁵

¹Industrial Technology Centre of Wakayama Prefecture, Wakayama, Japan; ²Graduate School of Engineering Science, Osaka University, Toyonaka, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ⁴Japan Atomic Energy Agency, Condensed Matter Research Unit, Sayo, Hyogo, Japan; ⁵Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan

A ladder compound NaV₂O₅ belongs to the quasi-one-dimensional spin system with the VO₅ chain lined along the b-axis. It shows the charge order (CO) transition with two V⁴⁺ and V⁵⁺ states at $T_c \sim 34$ K and has an insulating character below and above T_c . In order to investigate the electronic states near the Fermi level (E_F), we have carried out angle-resolved photoelectron spectroscopy (ARPES) for the momentum parallel to the b-axis at low excitation energy of about 10 eV. The measurement was performed at room temperature in order to avoid the charge up effect in the low temperature phase. The electronic states near E_F consist of V 3d state hybridized with O 2p state and clearly showed dispersive features. In the ARPES spectra, a broad peak was located at around $E_b = 1.3$ eV at $k_y/\pi = 0$, which splits into two peaks most separated around $k_x/\pi = 0.5$. These peaks converges around $k_x/\pi = 1$ again. The obtained spectral feature seems to be similar to that for Na_{0.96}V₂O₅ rather than that for NaV₂O₅ in the previous study [1].

[1] K. Kobayashi et al., PRL 80, 3121 [1998]; 82, 803 [1999].

3P048

Photoemission and soft X-ray absorption spectroscopies of quasi-one-dimensional BaVS₃

K Tobimatsu,¹ H Sato,² T Yamamoto,¹ M Arita,² M Sawada,² M Nakatake,² H Nakamura,³ A Tanaka,⁴ H Namatame,² M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan; ⁴ADSM, Hiroshima University, Higashi-Hiroshima, Japan

The quasi-one-dimensional BaVS₃ exhibits metal ($T > T_M$) - insulator ($T < T_M$) transition (MIT) at $T_M = 70$ K. Several models for MIT has been proposed, such as the charge density wave instability, the Mott insulator, and so on. In this study, we have, for BaVS₃ single crystals, carried out high-resolution photoemission spectroscopy (PES) at BL9A of HiSOR and the V 2p-3d soft X-ray absorption spectroscopy (XAS) at BL14 of HiSOR, in order to reveal its temperature-dependent electronic structure across MIT. From the $\rho_{//}$ -PES spectra near E_F , measured with the experimental configuration such that the spectra reflect the electronic states parallel to the V chain, we notice the low density of states (DOS) just at E_F even in the metallic phase, in consistent with the high resistivity. DOS around E_F decreases continuously with decreasing temperature from 280 to 20 K, and the spectral weight gradually transfers into ~ 0.4 eV region below E_F . No abrupt change is observed at T_M . Although the ρ_{\perp} -PES spectra show the similar behavior, DOS around E_F transfers into the deeper ~ 0.6 eV region and an amount of the transfer is smaller than that of the $\rho_{//}$ -case, reflecting the anisotropic electronic structure due to one-dimensional character. The V 2p-3d XAS spectra also exhibit a remarkable linear dichroism between $E//c$ and $E \perp c$. The temperature dependence is not detected in the $E//c$ -XAS spectra.

3P049

Temperature-dependent high-resolution angle-resolved photoemission study of the Shockley state in Cu(111)

D Hirayama,¹ H Iwasawa,² K Shimada,² M Arita,² J Jiang,¹ H Hayashi,¹ T Habuchi,¹ Y Aiura,³ H Namatame,^{1,2} M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³National Institute of Advance Industrial Science and Technology, Tsukuba, Japan

High-resolution angle-resolved photoemission spectroscopy (ARPES) enables us to clarify fine electronic structures such as a kink structure in the energy-band dispersion near the Fermi level (E_F). The kink structure indicates a coupling to bosonic excitations such as phonons or magnons. In this study, we have examined the temperature dependence of the kink structure derived from the electron-phonon interaction in the Shockley state of Cu(111). The Shockley state can be regarded as a typical two-dimensional Fermi Liquid with free-electron-like band dispersion and Fermi surface [1]. High-resolution ARPES experiments were performed on the helical undulator beamline of Hiroshima Synchrotron Radiation Center. We have set photon energy at $h\nu = 7$ eV, and total energy resolution at 5.5 meV. We could clearly observe the Shockley state as reported previously [1]. Based on the quantitative lineshape analyses, the electron-phonon coupling parameter was evaluated as $\lambda = 0.13 \pm 0.01$ at 10 K. We found that the magnitude of the kink structure decreases on heating which suggests a decay of the quasi-particle states. [1] F. Reinert *et al.*, Phys. Rev. B **63**, 115415 (2001).

3P050

Spin-doping effect on the electronic structure of Sr_{1-(x+y)}La_{x+y}Ti_{1-x}Cr_xO₃

T Saitoh,¹ H Iwasawa,^{1,2} K Kurahashi,¹ Y Nakano,¹ T Katsufuji,³ I Hase,⁴ K Shimada,² H Namatame,² M Taniguchi^{2,5}

¹Department of Applied Physics, Tokyo University of Science, Shinjuku-ku, Tokyo, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³Department of Physics, Waseda University, Tokyo, Japan; ⁴National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, Japan; ⁵Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan

Sr_{1-(x+y)}La_{x+y}Ti_{1-x}Cr_xO₃ can control the charge and spin degrees of freedom by changing the ratios of the two TM elements (Ti/Cr) or the two A-site ions (Sr²⁺/La³⁺); the conventional La³⁺ substitution for Sr²⁺ introduces electrons into the Ti 3d conduction band (by y), while Cr³⁺ ions can be introduced by replacing SrTiO₃ with LaCrO₃ (by x), which will be able to realize "spin doping" of S=3/2 local moment at Ti sites. A recent magnetic and transport study found an increasing ferromagnetic interaction with x in spite of a low T_C (below ~ 10 K) [1] and a photoemission study pointed out an important role of the large energy difference between the Ti 3d and the Cr 3d state [2]. A further detailed y-dependent electronic-structure study found that significant deviation from the band theory was actually caused by this large energy difference [3]. Here, we have investigated detailed spin-doping effects on the valence-band electronic structure. The Cr 3d spectral weight vs. x plot showed a proportional relationship, indicating that the expected control of the spin density by x as expected. The near- E_F weight, however, showed significant reduction with x. Because the band theory predicted the nearly constant weight, this should be attributed to strong Ti/Cr site disorder effects.

[1] J. Inaba *et al.*, Phys. Rev. B **72**, 052408 (2005). [2] H. Iwasawa *et al.*, Phys. Rev. Lett. **96**, 067203 (2006). [3] H. Iwasawa *et al.*, Phys. Rev. B **80**, 125122 (2009).

3P051

Fermi surface nesting and orbital dependent deformation in Mn-substituted $\text{Sr}_3\text{Ru}_2\text{O}_7$

ZH Zhu,¹ MA Hossain,^{1,2} G Levy,¹ D Fournier,¹ M Raichle,¹ Y Yoshida,³ A Bostwick,³ E Rotenberg,⁴ IS Elfimov,¹ A Damascelli¹

¹Department of Physics & Astronomy, University of British Columbia, Vancouver, BC, Canada; ²SIMES, SLAC, Stanford University, Menlo Park, CA, United States; ³National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; ⁴Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

We have studied the low-energy electronic structure of $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$ ($x=0, 0.05, 0.1$) by angle-resolved photoemission spectroscopy. As the system undergoes a metal-to-insulator transition driven by Mn impurities, the Fermi surface (FS) derived from the three t_{2g} orbitals of the parent compound starts losing the 2D character associated with the d_{xy} band. The resulting FS reduces to the 1D d_{zx} and d_{yz} bands derived states, and becomes fully nested. The doping evolution of the band dispersion points at the reduction of electron occupation of the d_{xy} band as the mechanism behind this orbital dependent deformation of the FS. Furthermore, the Mn-enhanced FS nesting might be connected to the emergence of the magnetic superstructure proposed for Mn-substituted $\text{Sr}_3\text{Ru}_2\text{O}_7$ on the basis of our resonant elastic soft X-ray scattering results [1]. [1] M.A. Hossain *et al.* arXiv:0906.0035 [2009].

3P052

Inverse-photoemission spectroscopy of iron-based superconductors $\text{NdFeAsO}_{0.7}$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

Y Utsumi,¹ H Sato,^{2,4} O Morimoto,² Y Nakashima,¹ A Ino,^{1,4} Y Aiura,^{3,4} A Iyo,^{3,4} H Kito,^{3,4} K Miyazawa,³ PM Shirage,³ H Eisaki,^{3,4} CH Lee,^{3,4} K Kihou,³ H Namatame,² M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan; ⁴Japan Science and Technology Agency, Transformative Research-Project on Iron Pnictide (JST-TRIP), Chiyoda, Japan

NdFeAsO and BaFe_2As_2 are parent compounds of iron-based superconductors and superconductivity appears with electron or hole doping. Both compounds have structural transition at 140-150 K from tetragonal structure in the high temperature phase to orthorhombic structure with an antiferromagnetic ordering in the low temperature phase. A great number of high-resolution angle-resolved photoemission experiments have been carried out for the iron-based superconductors, so far. In this study, we have investigated unoccupied electronic structure of $\text{NdFeAsO}_{0.7}$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ ($x = 0, 0.11$) by means of resonant inverse-photoemission spectroscopy (RIPES) in the low temperature phase. The Fe 3d states of $\text{NdFeAsO}_{0.7}$ were observed around 1 eV above E_F as a shoulder and exhibits almost no resonance in the Fe 3p-3d absorption region. On the other hand, the peak structure at 1 eV due to the Fe 3d states of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ shows a resonance behavior and the resonance seems to become remarkable with the Co doping. These results show that the unoccupied Fe 3d states of $\text{NdFeAsO}_{0.7}$ are almost itinerant, while those of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ have a localized character. The Nd 4d-4f RIPES for $\text{NdFeAsO}_{0.7}$ revealed that the Nd 4f components mainly contribute around 5 and 7 eV, and the Ba 5d and 4f states of BaFe_2As_2 are observed around 5 and 12 eV, respectively.

3P053

Polarization-dependent high-resolution angle-resolved photoemission spectroscopy of Pd(100)

H Hayashi,¹ K Shimada,² H Iwasawa,² J Jiang,¹ Y Aiura,³ H Namatame,² M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima, Japan; ³National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, Japan

Palladium (Pd) is a paramagnetic metal and located below ferromagnetic Nickel in the periodic table. Pd has the electronic states close to the magnetic instability, and is also well known as a hydrogen storage material. So far, there has been no report on the surface- and bulk-derived Fermi surfaces and detailed examination of the quasi-particle properties near the Fermi level. In this presentation, we report polarization-dependent high-resolution angle-resolved photoemission spectroscopy (ARPES) on Pd(100) single crystal. Experiments were done on the linear undulator beamline of Hiroshima Synchrotron Radiation Center (HiSOR). We have installed new ARPES system on a rotatable frame to change the s and p-polarization geometries. By changing the polarization geometry, we can selectively observe the initial states with odd or even symmetry with respect to the mirror plane. It is very effective for the multi-band systems where several Fermi surfaces exist close together. We have observed the bulk-derived Fermi surfaces of Pd in the Γ -XWK plane taken at $\hbar\nu = 160$ eV. We found good agreements between experimental and theoretical Fermi surfaces. Along the high symmetry lines, we could confirm that the energy-band dispersions were selectively observed depending on the symmetry with respect to the mirror plane. Taken at $\hbar\nu = 38$ eV, on the other hand, totally different Fermi surfaces were observed in the Γ -XWK plane. We found that they were derived from the surface electronic states.

3P054

Resonant soft X-ray scattering studies of multiferroic $Y(\text{Mn,Fe})_2\text{O}_5$ J Geck,¹ S Partzsch,¹ H Wadati,² E Schierle,³ E Weschke,³ R Kraus,¹ D Souptel,¹ GA Sawatzky,² B Büchner¹¹IFW Dresden, Dresden, Germany; ²University of British Columbia, Vancouver, Canada; ³Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Multiferroic materials with a cross-coupled ordering of electric and magnetic moments are rather rare in nature. Quite recently, however, a number of transition metal oxides were discovered, which not only show multiferroic behaviour, but also exhibit a strong magneto-electric coupling. Here we report resonant soft X-ray scattering (RSXS) and absorption experiments on multiferroic $Y\text{Mn}_{2-x}\text{Fe}_x\text{O}_5$. In addition, the lattice structure and the magnetic properties of single crystals with $x=0, 0.02, 0.07, 0.14$ were studied in detail. The undoped compound displays three phase transitions: Upon cooling incommensurate antiferromagnetic order sets in at 44K, which becomes commensurate and coexists with ferroelectric order at 40K. Finally, at 19K there is another transition to a low-temperature incommensurate antiferromagnetic phase, which is connected to a sharp drop of the electric polarization. Increasing the Fe-doping x results in a complete suppression of the incommensurate low-temperature phase for $x>0.07$. Our data also shows that Fe mainly occupies the pyramidal sites of the lattice. Single crystals with $x=0$ and $x=0.07$ were then studied by RSXS. The magnetic superlattice reflection of both samples exhibits strong resonances at the Mn $L_{2,3}$ -edge, as expected for ordered Mn-spins. More interestingly, we also observed a strong resonance at the O K-edge at this wave vector, revealing a spatial modulation of the oxygen valence states with the same periodicity as the magnetic order. The temperature dependent intensity of the superlattice peak on the O K-edge resonance tracks exactly the temperature dependence electric polarization, showing that this modulation of the valence states is directly connected to ferroelectricity. Our results reveal that, apart from ionic displacements, there exists an electronic contribution of the valence electrons to the electric polarization. This is in perfect agreement with a recent theoretical study. Interestingly, the superlattice reflection of the Fe-doped sample also resonates at the Fe $L_{2,3}$ -edge, which indicates that the doped Fe-sites take part in the electronic long-range order.

3P055

Experimental and theoretical investigation of electronic states and magnetism in N-doped rutile thin filmG Drera,¹ L Sangaletti,¹ M C Mozzati,² P Galinetto,² F Rossella,² F Bondino,³ M Malvestuto,³ Y A Diaz-Fernandez,² L Malavasi²¹Università Cattolica del Sacro Cuore, Brescia, Italy; ²Università degli Studi di Pavia, Pavia, Italy; ³IOM-CNR Laboratorio TASC, Basovizza (Ts), Italy

TiO_2 has been widely studied for its useful properties in many fields like photocatalysis, high-k gate insulator, gas sensing and recently as a closed-shell (formally d0) magnetic system; in particular the mechanism underlying d0 ferromagnetism (FM) are still under debate and present a challenge both from a theoretical and experimental point of view. Evidences suggest that doping impurities (if present), lattice defect or oxygen vacancies are involved in such behavior. In principle, nitrogen doping may allow to control both magnetism, by increasing defects and oxygen vacancies density, and photocatalytic behaviour by adding new state in the gap. In this work we study the magnetic and local electronic properties of undoped and N-doped TiO_2 thin films grown by RF sputtering in an Ar- N_2 controlled atmosphere. Both undoped and N-doped films display FM at room temperature (RT). In particular, N-doping results in a 5-fold increase of saturation magnetization as compared to undoped TiO_2 . By using a combination of GGA-PBE density functional theory calculations and element specific spectroscopic techniques, such as X-ray absorption and resonant photoemission (RESPES) at the Ti L-edge, we have been able to identify new electronic states related to N-doping. Both acceptor and donor levels appear in the rutile gap and add to electronic states due to oxygen vacancies already present in the undoped sample. On this basis, we discuss the possibility to relate the observed FM to an increase of the density of localized paramagnetic centers up to the percolation threshold, which triggers the observed RT long-range ferromagnetic ordering.

3P056

Electronic structure of perovskite-type nickelates studied by soft X-ray photoemission and absorption spectroscopyR Eguchi,^{1,2,4} A Chainani,² M Matsunami,^{1,2} M Oura,² Y Senba,³ H Ohashi,³ Y Okamoto,¹ Z Hiroi,¹ S Shin^{1,2}¹Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba, Japan; ²RIKEN SPring-8 Center, Sayo-gun, Hyogo, Japan; ³JASRI/SPring-8, Sayo-gun, Hyogo, Japan; ⁴Present address; The Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan

In previous work, we reported the out-of-plane and in-plane maps of the 3-D electron and hole Fermi surfaces of LaNiO_3 thin films using energy and angle-dependent photoemission measurements [1]. LaNiO_3 is a typical Fermi liquid metal among the perovskite nickelates $R\text{NiO}_3$. On the other hand, NdNiO_3 shows a clear first-order metal-insulator transition (MIT) at $T_{\text{MIT}} \sim 190$ K [2]. The photoemission studies of the polycrystalline samples were reported. However, across the MIT, a gradual change of the density of states at the Fermi level was observed despite a first order transition [3]. In this work, we study the electronic structures of NdNiO_3 thin films across the MIT using soft X-ray photoemission and absorption spectroscopy. These experiments were carried out using a photoemission system combined with a pulse laser deposition chamber at undulator beamline BL17SU, SPring-8. Optimum conditions for growing epitaxial NdNiO_3 films by pulsed laser deposition were obtained from studies of structure and electrical resistivity [4]. The angle-integrated photoemission spectra show changes across the MIT and an energy gap opens due to the reduced p - d hybridization in the low-temperature insulating phase. Simultaneously, the two peak structures of the Ni $2p$ absorption spectra also show changes depending on the temperatures, which indicates a clear first-order transition.

[1] R. Eguchi *et al.*, Phys. Rev. B **79**, 115122 (2009), [2] J.-S. Zhou *et al.*, Phys. Rev. Lett. **84**, 526 (2000), [3] I. Vobornik *et al.*, Phys. Rev. B **60**, R8426 (1999), [4] R. Eguchi *et al.*, J. Appl. Phys. **105**, 056103 (2009).

3P057

Application of charge transfer multiplet (CTM) theory to band edge states, and Tanabe-Sugano energy level diagrams to band edge defects in high-k gate dielectrics

G Lucovsky,¹ L Miotti,¹ K Paz Bastos¹¹Physics, NC State Univ, Raleigh, NC, United States

X-ray absorption and photoemission spectroscopy (SSRL) have been used to study conduction band, and O-vacancy defect states in ZrO_2 , Y_2O_3 and HfO_2 [1]. For the first time many-electron CTM theory has been applied to O K edge spectra. A similar approach using Tanabe-Sugano energy level diagrams is applied using an *equivalent d² state* model for O-vacancy defect features in the O K pre-edge regime. O K edge spectral assignments have generally neglected O 1s core hole localization [2]. Density functional theory studies of O-vacancy defects in HfO_2 and ZrO_2 have not taken proper account of the strongly correlated character of TM-atom d-states, yielding inherently flawed defect state energies. This leads to quantitative errors in interpreting defect state energies in spectroscopic ellipsometry studies [1]. A CTM theory has been applied to $M_{2,3}$ and O K edge spectra for nano-grain thin film ZrO_2 , Y_2O_3 , and HfO_2 . Tanabe-Sugano diagrams are used to assign spectral features in O K edge spectra to O vacancy defects using the d^2 model [3]. This approach has: (i) demonstrated the same energy sequencing of TM 4d- and 5s-states in Zr, Y and Hf oxide $M_{2,3}$ and O K edge spectra, and (ii) assigned the energies of d to d' transitions in pre-edge O vacancy defect states to d^2 high-spin states. The Tanabe-Sugano energy level assignments yield the same sequencing and symmetry assignments of O-vacancy defects in these three TM oxides [3]. The approach has also identified energies of O-vacancy *negative ion* electron traps at the conduction band edge.

[1] Lucovsky G, et al., Solid State Electronics 53, 1273 [2009].

[2] de Groot F, Kotani A. *Core level spectroscopy of solids* (Boca Ratan, CRC Press, 2008).

[3] Fugimori A, Minari F, Phys. Rev, B 30, 963 [1984].

3P058

Spectroscopic detection of spin-polarized bands and mixed valence for Ti and Sc in $GdSc_{1-x}Ti_xO_3$ for $x = 0.18$ and 0.25

K Paz Bastos,¹ L Miotti,¹ G Lucovsky¹¹Physics, NC State, Raleigh, NC, United States

Ti substituted for Sc in nano-grain and single crystal d^0 $GdScO_3$ films bonds in a trivalent state, Ti^{3+} , creating a mixed d^0 - d^1 oxide with composition-dependent transport properties; e.g., an insulator to metal transition for Ti content exceeding a percolation threshold of $\sim 16\%$ [1]. X-ray absorption spectroscopy at SSRL was used to study: (i) occupied electronic states of the Ti^{3+} atoms, (ii) O K edge conduction band and defect states, and (iii) 2p to 3d $L_{2,3}$ spectra. Comparisons between nano-grain films on Si substrates, and epi-thin films reveal differences in spin-up and spin-down correlation energy split bands. Second derivative pre-edge spectra indicate a strong spin-up band and a weaker spin-up band in epi-films. Randomly orientated nano-grains with dimensions < 3 nm result in a *single broad feature* spanning the width of the spin bands in the epi-films. O-atom vacancy defect features occur in pre-edge regime and scale with the Ti alloy fraction. Ti and Sc $L_{2,3}$ spectra indicate significant differences between spectra in alloy films above, and below the percolation threshold. Interpretations based on many-electron charge transfer multiplet [CTM] theory have identify a steady-state transfer of electrons from occupied Ti^{3+} to empty Sc^{3+} states resulting in Sc^{2+} states. This is by an intra-layer steady state hopping process, which results in a mixing of Ti^{4+} d^0 and Ti^{3+} d^1 features in Ti $L_{2,3}$ spectra. Spectral studies indicate conditions necessary for double exchange ferromagnetism are met by alloying Ti alloying above a percolation threshold of 16%, [2]. These are: (i) mixed valency of in-plane Ti and Sc atoms as detected in $L_{2,3}$ spectra, and (ii) hopping transport metallic conductivity as determined by electrical measurements.

[1] Lucovsky G, et al, Solid State Electronics 53, 1273 [2009].

[2] Cox PA, Transition metal oxides (Oxford Clarendon, 1992).

3P059

Spectroscopic detection of Ti and Sc Fano and defect state resonances in high-resolution $L_{2,3}$ resonant photoemission spectroscopy (RPES) measurements

L Miotti,¹ K Paz Bastos,¹ G Lucovsky¹¹Physics, NC State Univ, Raleigh, NC, United States

In valence band photoemission spectroscopy when the incident photon energy resonates with occupied valence band and d-states states, the photoemission displays either resonantly enhanced features, or Fano resonances [1]. Resonances for are reported for Sc and Ti 2p core level $L_{2,3}$ spectra in $GdScO_3$ alloyed with Ti. Ti 2p core level spectra are compared with RPES studies of thin film d^0 TiO_2 , and single crystal d^1 $LaTiO_3$. Substitution of Ti for Sc in preovskite Sc-O planes yields a Ti^{3+} state, converting the d^0 host oxide to a mixed d^0 - d^1 alloy with an insulator to metal transition for Ti concentrations of 18 and 25% [2]. Fano and enhancement resonances are observed at the same incident photon energies, but are associated with different regions of the valence band spectrum determined by energy analysis of photo-emitted electrons. Spectral measurements were made at beam-lines 13-2 and 10-1 at SSRL. Both types of resonances were detected in Ti $L_{2,3}$ and Sc $L_{2,3}$ spectra of the 18% and 25% alloys. These are distinguished by different energies of occupied continuum states within the valence band, or localized Ti alloy atom states above the valence band edge. The Ti $L_{2,3}$ enhanced resonance with the Ti^{3+} occupied ground state is above the valence band edge, and the four Fano resonances are within the valence band continuum states associated with Ti molecular orbital bonding states. The $L_{2,3}$ spectra of Sc also indicate four Fano resonances. These are within the valence band continuum and are associated with Sc t_{2g} - and e_g -bonding states in the both the L_3 and L_2 spectral components of the Sc $L_{2,3}$ edge.

[1] de Groot F, Kotani A. *Core level spectroscopy of solids* (Boca Ratan, CRC Press, 2008).

[2] Lucovsky G, et al, Solid State Electronics 53, 1273 [2009].

3P060

Study of charge/orbital state in layered perovskite manganite $\text{Nd}_{2-x}\text{Sr}_x\text{MnO}_4$ by resonant X-ray scattering

M Kubota,¹ Y Oohara,² D Akahoshi,³ H Kuwahara³

¹KEK PF, Tsukuba, Japan; ²ISSP, Kashiwa, Japan; ³Sophia University, Tokyo, Japan

We have newly developed an apparatus for soft X-ray scattering in materials science research fields such as strongly-correlated electron systems (SCES). The scattering equipment has been constructed at the BL16A undulator beamline, where fast polarization switching at a frequency of ~ 10 Hz will be available in 2010. Since the beamline BL16A covers the energy region of 200- 1500 eV, we reveal the significance of the hybridization between the 3d electronic state and the oxygen electronic state in the transition metal oxides. We have performed soft X-ray scattering on layered perovskite manganite $\text{Nd}_{2-x}\text{Sr}_x\text{MnO}_4$ ($x=2/3$), which show orbital/charge ordered states in the two dimensional system ($T_c \sim 270\text{K}$). The satellite peaks appear at Mn absorption edge below $\sim 250\text{K}$ at $(1/6, 1/6, 0)$. The magnitude gradually increases, with lowering temperature. The correlation length remains short ranged. The satellite peaks at O absorption edge are also observed. In the near future, we will establish automatization of both the centering adjustment of the sample position. We will further revise the equipment to detect inelastic scattering signals.

3P061

Exploring polarization dependencies in XAS on single layer (Pb,La)-Bi2201 beyond the common view of cuprate

B Müller,¹ A K Ariffin,¹ R Mitdank,¹ L Dudy,¹ A Krapf,¹ H Dwelk,¹ C Janowitz,¹ R Manzke¹

¹Humboldt University, Berlin, Germany

Using X-ray absorption spectroscopy (XAS) in cuprates at the CuL_3 and OK edge, the contributions of Cu and O to the electronic structure can be investigated. While previously only out-of-plane polarization dependencies were studied, now a polarization dependence within the CuO_2 plane has been detected in the single layer Bi cuprate (Pb,La)-Bi2201. Spectral features related to the Zhang-Rice singlets are modulated with varying azimuthal angle. The characteristics of the angular distribution move beyond the $d_{x^2-y^2}$ symmetry expected from single band models which incorporate only $\text{Cu}3d_{x^2-y^2}$ and $\text{O}2p_{x,y}$ into the description of the electronic structure. The samples studied had varying combinations of La and Pb, and thus, different hole concentrations. Therefore, almost the whole superconducting dome was studied. This systematic enables the discussion of some characteristics that support theories questioning Zhang-Rice singlets.

3P062

Photoemission of a doped Mott insulator: spectral weight transfer and absence of metallic state

M Sing,^{1,2} S Glawion,¹ M Schlachter,¹ MR Scholz,¹ K Goss,¹ J Heidler,¹ G Berner,¹ R Claessen¹

¹Cologne University, Cologne, Germany; ²Wuerzburg University, Wuerzburg, Germany

In the attempt to understand the mechanism which leads to high-temperature superconductivity in the cuprates it is widely accepted as the least common denominator of this material class that they are doped Mott (or charge-transfer) insulators. Hence, the question how the electronic structure of a Mott insulator develops upon doping is of fundamental interest. TiOCl is a prototypical quasi-one-dimensional Mott insulator with a d^1 configuration. In this respect it represents the electron analogue to the almost full d shell with one single hole in the cuprates. Employing photoelectron spectroscopy, we observe a spectral weight transfer between the lower Hubbard band and the additional weight upon electron-doping which is a hallmark of correlated bands. In contrast, the absence of a metallic quasiparticle peak is traced back to one-particle effects. Against the background of recent density-functional calculations [1], we identify alkali-metal doped TiOCl as an alloy Mott insulator, where the alloy sites with changed orbital energies are induced electrostatically by the intercalants [2].

[1] Y.-Z. Zhang, K. Foyevtsova, H. O. Jeschke, M. U. Schmidt, and R. Valenti, Phys. Rev. Lett. 104, 146402 [2010].

[2] M. Sing, S. Glawion, M. Schlachter, M. Scholz, K. Goss, J. Heidler, G. Berner, and R. Claessen, arXiv:0905.1381v2.

3P063

Temperature dependent quasiparticle renormalization in nickelR Ovsyannikov,¹ J Sánchez-Barriga,¹ J Fink,¹ HA Dürr²¹Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany; ²SLAC, Stanford University, Stanford, United States

One of the fundamental consequences of electron correlation effects is that the bare particles in solids become 'dressed' with an excitation cloud resulting in quasiparticles. Such a quasiparticle will carry the same spin and charge as the original particle, but will have a renormalized mass and a finite lifetime. The properties of many-body interactions are described with a complex function called self energy which is directly accessible to modern high-resolution angle resolved photoemission spectroscopy (ARPES). Ferromagnetic metals like nickel or iron offers the exciting possibility to study the spin dependence of quasiparticle coupling to bosonic modes. Utilizing the exchange split band structure as an intrinsic 'spin detector' it is possible to distinguish between electron-phonon and electron-magnon coupling phenomena. In this contribution we will discuss a spin dependent quasiparticle band structure of Ni (111) studied with high resolution angle resolved photoemission spectroscopy. At low temperatures (50 K) a renormalization of quasiparticle energy and lifetime indicative of electron-phonon coupling is observed in agreement with literature [1]. With increasing temperature we observe a decreasing quasiparticle lifetime at the Fermi level for all probed minority spin bands as expected from electron phonon coupling. Surprisingly the majority spin states behave differently. We actually observe a slightly increased lifetime at room temperature. The corresponding increase in Fermi velocity points to a temperature dependent reduction of the majority spin quasiparticle renormalization. [1] M. Higashiguchi et al., Phys. Rev. B 72, 214438 (2005)

3P064

Metal-insulator transitions and dimensional crossover in $[\text{LaMnO}_3]_{2n} / [\text{SrMnO}_3]_n$ manganite superlattices investigated by MBE-ARPESKM Shen,¹ EJ Monkman,¹ C Adamo,² DG Schlom²¹Department of Physics, Cornell University, Ithaca, NY, United States; ²Department of Materials Science and Engineering, Cornell University, Ithaca, NY, United States

We present angle-resolved photoemission spectroscopy (ARPES) studies of the electronic structure of $[\text{LaMnO}_3]_{2n} / [\text{SrMnO}_3]_n$ superlattices using a new technique which combines oxide molecular beam epitaxy (MBE) growth and ARPES. Oxide interfaces and superlattices present a new playground for investigating and controlling the properties of correlated electronic materials. $[\text{LaMnO}_3]_{2n} / [\text{SrMnO}_3]_n$ superlattices exhibit a variety of electronic states as a function of layer thickness n and temperature, including a transition from metallic ($n < 3$) to insulating behavior for ($n \geq 3$). We present ARPES measurements of the Fermi surface and remnant Fermi surface for metallic and insulating superlattices and compare these to calculations based on density functional theory. We will discuss the 2D quantum confinement of mobile carriers to the interfaces with increasing n , and the suppression of spectral weight at the Fermi level across the metal-insulator transition. In addition, we will present the first high-resolution ARPES measurements of the metal-insulator transition in $\text{Eu}_{1-x}\text{Gd}_x\text{O}$ and the correlated 4d ferromagnet SrRuO_3 which have been made possible by the development of our integrated MBE-ARPES system.

3P065

Temperature-induced valence transition of EuPd_2Si_2 studied by hard X-ray photoelectron spectroscopyK Mimura,¹ T Uozumi,¹ T Ishizu,¹ S Motonami,¹ H Sato,² Y Utsumi,³ S Ueda,⁴ A Mitsuda,⁵ K Shimada,² Y Taguchi,¹ Y Yamashita,⁴ H Yoshikawa,⁴ H Namatame,² M Taniguchi,^{2,3} K Kobayashi⁴¹Department of Mathematical Sciences, Osaka Prefecture University, Sakai, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan;³Department of Physical Science, Hiroshima University, Higashi-Hiroshima, Japan; ⁴NIMS Beamline Station at SPring-8, National Institute of Materials Science, Hyogo, Japan;⁵Department of Physics, Kyushu University, Fukuoka, Japan

Electronic structure of EuPd_2Si_2 , which undergoes an abrupt valence transition at around 160 K: the Eu mean valence changes from 2.8 below 130 K to 2.3 above 180 K [1], has been investigated by temperature-dependent hard X-ray photoelectron spectroscopy (HX-PES). The HX-PES experiments were performed at the undulator beamline BL15XU of SPring-8. The temperature-dependent HX-PES spectra clearly showed the valence transition with abrupt changes in the divalent and trivalent Eu 3d components. The Eu 3d spectral shape, especially the drastic change in trivalent Eu 3d feature with temperature, could not reproduced by the atomic calculation. Therefore, we have done calculations based on the Anderson model in which the hybridization of the trivalent Eu 4f electrons with the conduction electrons and the f-f hybridization between the divalent and trivalent Eu with anisotropic symmetry are taken into account. According to the model calculation, the change in the trivalent Eu 3d spectral shape through the valence transition is closely related to the degree of admixture of the excitation state ($J = 1, 2$) and the ground states ($J = 0$) of trivalent Eu. [1] See for example, E.V. Sampathkumaran et al., J. Phys. C 14, L237 (1981).

3P066

Regularities of growth of carbon metal-containing nanoforms in nanoreactorsIN Shabanova,¹ NS Terebova¹¹Physicotechnical Institute of the Ural Division of the Russian Academy of Sciences, Izhevsk, Russian Federation

For conducting the systematic investigations of the electronic structure of nanosystems, nanostructure model specimens were synthesized, in which transition metals from IV, V and VI periods with different number of d electrons and sp elements from II and III periods with different number of p electrons were used as modifiers. This allowed to develop the method of X-ray photoelectron spectroscopy for its application for monitoring and investigating the structure of nanoforms, to develop a model for the determination of the forms of the synthesized nanostructures. The activity of the nanostructure synthesis was studied depending on the additions of sp elements into the nanoreactors of polymer matrices. Based on the conducted X-ray photoelectron investigations, a conception was developed of studying the growth of nanostructures of a definite form and their properties by the interaction of initial components and about the possibility of the formation of the hybridized chemical bond of d electrons of metal atoms with p electrons of sp element atoms. A method was developed for the determination of the magnetic moment of d metals and the change of the distance between the metal atoms and the sp-element atoms by the parameters of the X-ray photoelectron spectra of transition metals, which allows to establish the degree of the hybridization of valence electrons in the chemical bond of neighboring atoms (Me-X). Based on the investigations, the regularities were established which provide the development of new trends in the synthesis of nanostructures with unique properties.

3P067

Correlation between electronic structures and photocatalytic activities of nanocrystalline-(Au, Ag, and Pt) particles on the surface of ZnO nanorodsJW Chiou,¹ SC Ray,² WF Pong,² JH Guo³¹Department of Applied Physics, National University of Kaohsiung, Kaohsiung, Taiwan; ²Department of Physics, Tamkang University, Tamsui, Taiwan; ³Advanced Light Source, LBNL, Berkeley, United States

O K-, Au, Ag and Pt L_{3} -edge X-ray absorption near-edge structure (XANES), X-ray emission spectroscopy (XES) and scanning photoelectron microscopy (SPEM) measurements have been performed to study the correlation between the electronic structures and photocatalytic activities of nanocrystalline (nc)-(Au, Ag, and Pt) particles on the surface of ZnO nanorods (ZnO-NRs). The O K-edge XANES spectra reveal greater occupation of the O 2p orbitals, i.e. a greater negative effective charge of the O ions, in nc-Pt/ZnO-NRs than of nc-(Au, Ag)/ZnO-NRs. This result suggests that nc-Pt particles have weaker photocatalytic activities than those of nc-(Au, Ag) particles on the surface of ZnO-NRs. Well-defined bandgaps of nanoparticle-coated ZnO-NRs increase in the order Au (3.3 eV)- Pt (3.5 eV)- Ag (3.6 eV), which can be correlated with an increasing Pauling's electronegativity and a reduction of the screening effect. The valence-band SPEM measurement of nc-(Au, Ag, and Pt)/ZnO-NRs does not support the general argument that the Fermi levels of the (Au, Ag)/semiconductor composites are shifted toward the conduction-band edge relative to that of the Pt/semiconductor composite.

3P068

Wavelet investigation of EXAFS data for thin films of Mn doped Si based diluted magnetic semiconductorsZ Pan,¹ Y Feng,¹ Z Xie,¹ J Ye,¹ S Wei,¹ Z Wu¹¹National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui, China

The Morlet wavelet transformation was used to analyze Mn K-edge extended X-ray absorption fine structure (EXAFS) spectra of Mn doped Si based diluted magnetism semiconductor (DMS) thin films growth by the magnetron co-sputtering method at low temperature. EXAFS data show that the Mn-Mn scattering path can be distinguished by the Mn-Si scattering path in the spectra of Mn_xSi_{1-x} DMS thin films. In all DMS thin films investigated, Mn atoms fill Si sites without occurrence of Mn-Si compounds which on the contrary are present in their annealed analogues. We point out that the low-concentration Mn doping samples are characterized by a more symmetric structure respect to the high-concentration one having similar bond-lengths inside both Mn-Mn and Mn-Si coordination shells.

3P069

High-resolution photoemission spectroscopy of one-dimensional Pt complex [Pt₂(MeCS₂)₄]₂ClO₄

T Habuchi,¹ M Mitsumi,² K Shimada,³ H Iwasawa,³ J Jiang,³ H Hayashi,¹ D Hirayama,¹ H Namatame,³ M Taniguchi^{1,3}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Material Science, University of Hyogo, Kamigori, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan

One-dimensional (1D) metal, which is often referred to as the Tomonaga-Luttinger liquid (TLL), has attracted much interest for its unusual physical properties. Recently, high-quality single crystalline Pt complex, [Pt₂(MeCS₂)₄]₂ClO₄, has been obtained. As the 1D metallic Pt chain is coordinated by the insulating organic ligands, the chains are expected to be electrically isolated. In this study, we have done temperature-dependent high-resolution photoemission spectroscopy (PES) of the Pt complex for the first time, to directly reveal its electronic state. High-resolution PES experiments were performed on the linear undulator beamline of HiSOR. We found that the spectral intensity was suppressed near the Fermi level, and the energy dependence of the spectral intensity can be reproduced reasonably well by $\rho(\omega) = C|\omega|^0$. It indicates that the electrons in the Pt complex behave as TLL.

3P070

Germanium nanowires: the application of synchrotron radiation to the study of nanomaterials.

MJ Ward,¹ TK Sham¹

¹Department of Chemistry, The University of Western Ontario, London, Ontario, Canada

The study of one-dimensional (1D) inorganic semiconducting nanostructures such as wires, belts, tubes, ribbons, and rods has recently become the focus of intense research because of their potential application in nano-scale electronic, optical, and sensing devices.¹ Thus it has become of equal, if not greater importance, to develop techniques for studying the aforementioned desirable effects of these materials. Germanium nanomaterials are of particular interest since germanium has a higher carrier mobility and larger bohr-exciton radius than silicon which makes these materials well suited for use as nanoscale field effect transistors (nano-FET's) and tunable far-IR detectors respectively.^{2,3,4} We used X-ray absorption spectroscopy (XAS) and X-ray excited optical luminescence (XEOL) to study the bulk and surface electronic properties, and the optical properties of germanium nanomaterials. We have demonstrated that by studying both the fluorescence yield (FY) and the total electron yield (TEY) channels for the Ge L_{2,3}-edge we can track changes in the surface oxide thickness of germanium nanowires. We have used XAS-XEOL experiments to study the origin and energy dependence of the bright blue luminescence observed for germanium nanowires. Research at UWO is supported by NSERC, CFI, OIT, and CRC. Synchrotron experiments were conducted at the Canadian Light Source.

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3P071

Particular kind of dispersive structures of TlSe investigated by angle-resolved photoemission spectroscopy

S Motonami,¹ K Mimura,¹ T Ishizu,¹ S Kawada,¹ M Arita,² K Wakita,³ N Mamedov,⁴ S Hamidov,⁴ G Orudzhev,⁴ H Namatame,² M Taniguchi,² Y Taguchi¹

¹Department of Mathematical Sciences, Osaka Prefecture University, Sakai, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³Department of Electrical, Electronics and Computer Engineering, Chiba Institute of Technology, Narashino, Japan; ⁴Institute of Physics, Azerbaijan National Academy of Science, Baku, Azerbaijan

Electronic band structure of heavy-elemental chalcogenide TlSe with quasi one-dimensional crystalline structure has been investigated by means of high resolution angle-resolved photoemission spectroscopy (ARPES) in order to check for dispersive structures like the Dirac cone observed in the surface bands of Bi₂Se₃ [1]. The ARPES experiments were performed at the beamline BL-9A of HiSOR. Two linear dispersive structures which are not reproduced in band calculations for the bulk [2] were observed only in the energy band along Γ -N direction perpendicular to the chains. These dispersions form a cross-type structure which is centered at the Γ point and extends along Γ -H-T direction parallel to the chains. The observed structure differs from the cone-type structure disclosed for Bi₂Se₃ [1] and reflects, in our opinion, the surface dimensionality of TlSe. TlSe is one-dimensional, while Bi₂Se₃ is two-dimensional. The energy position of the cross-type structure shows the linear excitation photon energy dependence. Therefore we believe that in fact the disclosed dispersive structures in ARPES of TlSe are bound to the conduction bands and the ARPES detects the joint density of states.

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3P072

Soft X-ray absorption spectroscopy study of Mo-rich $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ perovskite oxides ($0.5 \leq x \leq 1$)

JS Kang,¹ JH Hwang,¹ DH Kim,¹ S Kolesnik,² B Dabrowski,² BG Park,³ JY Kim,³ J Lee,⁴ B Kim,⁴ BI Min⁴

¹Physics, The Catholic University of Korea, Bucheon, Republic of Korea; ²Physics, Northern Illinois University, DeKalb, Illinois, United States; ³Pohang Accelerator Laboratory, POSTECH, Pohang, Republic of Korea; ⁴Physics, POSTECH, Pohang, Republic of Korea

Doping of the Mn site in RMnO_3 -type perovskite oxides with different transition-metal elements exhibit the interesting phenomena, such as CMR, the metal-insulator transition, and the rich phase diagram. In this aspect, it is interesting to study $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ since the substitution of Mo ions for Mn ions would yield a large variation in the valence states of Mn ions due to the high valency of a Mo ion (Mo^{5+} or Mo^{6+}), while the structural disorder in the Mn lattice is relatively small. In this work, we report the electronic structures of $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ in the Mo-rich concentration regime ($0.5 \leq x \leq 1$), which were investigated by employing soft X-ray absorption spectroscopy (XAS). We have measured both the Mn 2p and Mo 3p XAS spectra of $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ for $x \geq 0.5$, and performed the configuration interaction cluster model calculations. The Mn 2p XAS spectra of $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ for $x \geq 0.5$ indicate that the valance states of Mn ions are nearly divalent and that they remain nearly unchanged for $x \geq 0.5$. On the other hand, the Mo 3p XAS spectra of $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ are rather broad and weak, but they show some changes with x . Based on this work, we can understand the electronic structures of $\text{SrMn}_{1-x}\text{Mo}_x\text{O}_3$ in the Mo-rich regime ($0.5 \leq x \leq 1$).

3P073

Magnetic anisotropy and interface magnetism of Fe and Pd/Fe ultra-thin films on Pd(001) investigated by X-ray magnetic circular dichroism spectroscopy

T Ueno,¹ M Sawada,² K Furumoto,¹ T Tagashira,¹ A Kimura,¹ H Namatame,² M Taniguchi^{1,2}

¹Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan

Various kinds of coupling of 3d ferromagnetic transition metals and 4d or 5d noble metals are known to generate several types of ferromagnetic ordered alloy, such as L_{10} , FePt, CoPt, and FePd. Palladium is 4d paramagnetic element on the verge of ferromagnetism because of its high density of states right at the Fermi energy. Therefore it is expected that the electronic structure and magnetism of Fe is strongly modified via Fe 3d - Pd 4d orbital hybridization in Fe/Pd system. As far as we know, only a few studies about magnetism of submonolayer Fe on Pd(001) and Pd covered Fe ultra-thin films have been reported so far. In order to reveal the magnetic anisotropy and the interface magnetism of Fe/Pd system, we prepared bare and Pd covered Fe monolayer (ML) films on Pd(001) and performed X-ray magnetic circular dichroism (XMCD) experiments. Sample preparation and XMCD experiments were *in situ* carried out at the XMCD end station of HiSOR-BL14 of Hiroshima Synchrotron Radiation Center. Fe thickness dependent XMCD at Fe $L_{2,3}$ edges revealed that the SRT occurs in Fe/Pd(001) at the critical Fe thickness. Pd/Fe/Pd(001) ultra-thin films exhibits in-plane magnetic anisotropy. Fe 3d spin and orbital magnetic moments in Fe ultra-thin films are enhanced compared to those of the bulk bcc Fe. We have observed Pd $M_{2,3}$ XMCD spectra and revealed that the magnetic moments are induced on Pd atoms in Fe/Pd interface. It can be considered that these results are originated from the Fe 3d - Pd 4d orbital hybridization.

3P074

Comparison of the electronic structure of $\text{LnBaCo}_2\text{O}_{5+\delta}$ (Ln = Gd, Dy, $\text{Dy}_{1-x}\text{Tb}_x$, Ln-112) and $\text{LnBaCo}_4\text{O}_7$ (Ln = Yb, Ln-114) single-crystal surfaces using resonant photoemission

HM Rafique,¹ WR Flavell,¹ AG Thomas,¹ KL Syres,¹ SN Barilo,² SV Shiryaev,² DMP Holland,³ AER Malins,³ G Miller,³ VR Dhanak³

¹The Photon Science Institute, The University of Manchester, Manchester, Great Britain; ²The Institute of Solid State and Semiconductor Physics, Belarussian Academy of Science, Minsk, Belarus; ³STFC Daresbury Laboratory, Daresbury, Warrington, Cheshire, Great Britain

$\text{LnBaCo}_2\text{O}_{5+\delta}$ (Ln-112) and $\text{LnBaCo}_4\text{O}_7$ (Ln-114) are correlated Co oxides that show potentially useful magnetic properties. The 'double perovskites' $\text{LnBaCo}_2\text{O}_{5+\delta}$ (Ln = lanthanide, $0 \leq \delta \leq 1$) show giant magnetoresistive behaviour in narrow composition ranges around $\delta = 0.5$ (Co(III)), a range of poorly understood spin state transitions, and a temperature-dependent metal-insulator (MI) transition. Co(III) is present in two environments, octahedral and pyramidal. The Kagome antiferromagnet $\text{LnBaCo}_4\text{O}_7$ contains no octahedral Co - instead sheets of CoO_4 tetrahedra are present. A comparison of the electronic structure of Ln-112 and Ln-114 single-crystal surfaces has been made using resonant photoemission. This shows that in both cases, the states close to the Fermi energy have mixed Co 3d/O 2p character. Comparison of the photoemission results for the two systems allows identification of the spectral signal due to low spin octahedral Co(III) in Ln-112. High resolution spectra reveal the presence of the MI transition in Ln-112 in the 300-400 K temperature range. The gradual changes in the spectral profile of the low energy states with temperature rule out a sudden 'high spin-low spin' switch as the mechanism of the MI transition. They are instead consistent with a gradually shifting equilibrium between low, intermediate and high spin states.

3P075

Coupled magnetic multilayer systems studied by resonant reflectivity in the XUV range

P Grychtol,¹ R Adam,¹ S Valencia,² S Cramm,¹ DE Bürgler,¹ CM Schneider¹

¹IFF-9, Forschungszentrum Juelich, Juelich, Germany; ²BESSY, Helmholtz-Zentrum-Berlin, Berlin, Germany

Mono- and polycrystalline multilayer systems of the spin-valve type based on transition metals (Fe, Co and Ni) were fabricated by sputtering and thermal evaporation in an ultra-high vacuum. They have been investigated both by measurements of the longitudinal MOKE in the visible range and by reflectivity measurements of resonantly scattered p-polarized light at the synchrotron in the XUV. By employing a transversal MOKE geometry close to the Brewster angle at the M absorption edges of Co and Ni (60.2eV and 67.5eV, respectively) a magnetic contrast as large as 80% for Co and 20% for Ni could be obtained upon magnetization reversal. In order to map the magnitude of the dichroism, angular and energy dependent scans of the magnetic asymmetry were performed and compared with magneto-optical simulations of the multilayer response. Element-selective hysteresis loops were recorded as a function of the interlayer thickness and reflect the switching behaviour of individual ferromagnetic layers as a function of the interlayer coupling. The magneto-optical response of a multilayer system to a laser-induced magnetic pulse excitation results in element-specific oscillations located in a frequency range of 3GHz to 6.5GHz. They can be associated with precessional magnetization dynamics of individual ferromagnetic layers. Our results demonstrate the feasibility of element- and layer-specific magneto-dynamic studies on magnetic multilayers by means of resonant reflectivity in the XUV.

3P076

Change in electronic structure within martensitic phase of Ni₅₀Mn₃₈Sn₁₂

S Singh,¹ G Adhikary,² D Biswas,² K Maiti,² C Biswas¹

¹Department of Material Sciences, S. N. Bose National Centre for Basic Sciences, Kolkata, India; ²Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, India

The Ni₅₀Mn₃₈Sn₁₂ is the Heusler alloy that show martensitic transition upon cooling. The electronic structure is considered to be the driving force for stabilizing the martensitic phase. Here the electronic structure of Ni₅₀Mn₃₈Sn₁₂ has been probed as a function of temperature by photoelectron spectroscopy using He I source. Within the martensitic phase, the valance band shows interesting changes as a function of temperature. At room temperature (RT) it is in paramagnetic martensitic phase. The valance band exhibits two peaks at 1 eV and 1.6 eV binding energy (BE). The ferromagnetic martensite is obtained below 170K. The valance band at 140 K is dominated by a broad peak at 1.24 eV BE. On further cooling in martensitic phase down to 9 K, the valance band shows two features at 1eV and 1.6 eV. The valance band is similar to that of paramagnetic martensitic phase. The density of states (DOS) near Fermi energy as a function of temperature is also worth noting. With the decrease in temperature within the martensitic phase the DOS near Fermi energy is decreasing giving rise to a pseudogap like feature. The origin of this change can be magnetic or structural. The changes within the martensitic phase with temperature have been explained in terms of resistivity, magnetization, magnetoresistance and neutron diffraction. The analysis implies the origin of changes to be magnetic in nature.

3P077

Extreme vacuum ultraviolet magnetic linear dichroism investigations at Ni M-edge of NiO thin film

S Xi,¹ M Cui,¹ J Zhao,² K Zhou,³ D Yang¹

¹Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China; ²Math. & Phys. Dept., Beijing Technology and Business University, Beijing, China; ³Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

Extreme vacuum ultraviolet (EUV) magnetic linear and circular dichroism (EUVMLD&EUVMCD), which focus on the M-edge of transition metals usually, have been providing great opportunity for investigating magnetic systems. It is the same as L-edge XMCD and XMLD that EUVMCD can study the magnetic properties of metallic state metals for its ferromagnetism, while EUVMLD has its advantage in the oxides which are usually antiferromagnetic. Comparing with L-edge, a better signal-to-noise ratio at M-edge can be achieved due to much narrower lifetime broadening. In this work we carried out the EUVMLD experiments at M edge of Nickel in NiO thin film on beam line 3W1B at Beijing Synchrotron Radiation Facility (BSRF). (98 ± 1)% linearly polarized X-rays are provided using Mo/Si multilayer mirror polarizer at Brewster's angle (49.5 degree). All measurements were carried out in the normal incidence at T= 298 K in transmission mode, under an external magnetic field of 2800 Gs. We obtained two sets of transmission spectra with linearly polarized X-rays perpendicular and parallel to the applied magnetic field, respectively. The observed spectra showed significant difference between them. The enormous dichroism signal demonstrates the feasibility of EUVMLD at M edge of Transition-Metal at our beam line. Further investigations of the theory and experiment such as the comparisons with the results from L-edge XMLD or XMCD are on the way.

3P078

Strong K-edge magnetic circular dichroism detected by resonant inelastic X-ray scattering

A Juhin,¹ M Sikora,² TS Weng,³ P Sainctavit,⁴ C Detlefs,³ FMF de Groot,¹ P Glatzel³

¹Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands; ²Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Kraków, Poland; ³European Synchrotron Radiation Facility, Grenoble, France; ⁴Institut de Minéralogie et de Physique des Milieux Condensés, Paris, France

X-ray magnetic circular dichroism (XMCD) is a powerful tool for the element-specific study of the magnetic structure of complex systems. It enables at spin-orbit split absorption edges to determine spin and orbital magnetic moments by means of sum rules. The magnetic moments of 3d transition metals (TM) are generally studied at the L_{2,3} absorption edges using soft X-rays whose short penetration depth limits the number of possible applications. Hard X-rays are used at the K-edge but the very weak XMCD signal and the absence of spin-orbit split edges do not allow for a detailed quantitative interpretation. We show that XMCD combined with resonant inelastic scattering (RIXS) of hard X-rays at the K pre-edge of Fe in magnetite yields a dichroic signal that is of the same order of magnitude as L-edge XMCD. Crystal field multiplet calculations are in good agreement with experiment and revealed that the effect arises from intraatomic 2p-3d Coulomb repulsions, 2p and 3d spin-orbit coupling. A strong MCD effect in the hard X-ray range opens new opportunities for earth sciences and condensed matter physics, allowing for truly bulk sensitive, element- and site-selective measurements of 3d TM magnetic moments and their ordering under demanding sample environments such as high pressure cells.

3P079

Soft X-ray photoemission study on antiperovskite manganites Mn₃Cu_{1-x}Ga_xN (x = 0, 0.5)

Y Miyata,¹ K Mima,¹ R Yamaguchi,¹ A Yamasaki,² A Higashiya,³ T Muro,⁴ K Terashima,¹ K Takenaka,⁵ A Ozawa,⁵ T Inagaki,⁵ S Imada¹

¹Ritsumeikan University, Kusatsu, Shiga, Japan; ²Konan University, Kobe, Hyogo, Japan; ³WINTEC, Wakayama, Wakayama, Japan; ⁴JASRI/SPring-8, Sayo, Hyogo, Japan; ⁵Nagoya University, Nagoya, Aichi, Japan

Antiperovskite manganese nitrides Mn₃XN (A = Zn, Ga, etc) are well known for their sudden contraction on heating at certain temperature ranges [1], so called negative thermal expansion (NTE). Since this NTE is accompanied by the formation of antiferromagnetic order, it is considered to be a magnetovolume effect, where the crystal and the magnetic structures are closely related with each other. Unlike other Mn₃XN, Mn₃CuN does not show NTE. Instead, it shows a ferromagnetic phase transition at T_c = 143 K accompanied by a cubic-to-tetragonal structural deformation on cooling [2]. Interestingly, a partial substitution of Ga for Cu effectively suppresses the ferromagnetic ordering, and Mn₃Cu_{0.5}Ga_{0.5}N clearly shows NTE just as the other Mn₃XN. To discuss the relationship between crystal and magnetic structures, we have performed soft X-ray photoelectron spectroscopy (SXPS) on Mn₃Cu_{1-x}Ga_xN (x = 0, 0.5) at BL27SU in SPring-8. We have found that the Mn 3d peak in the vicinity of Fermi level becomes less sharper through Ga substitution. This change is consistent with the result of band calculation using KKR-CPA method. From these results, we argue that the Ga substitution for Cu weakens the hybridization between Cu 3d and Mn 3d electrons, which suppresses the exchange splitting of Mn 3d bands.

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3P080

Electronic structure, magnetic and dielectric properties of the spin-chain compound NaCu₂O₂

P Leininger,¹ M Rahlenbeck,¹ M Raichle,¹ B Bohnenbuck,¹ A Malyuk,² C Lin,¹ B Keimer,¹ E Weschke,² E Schierle,² S Seki,³ Y Tokura,³ J Freeland⁴

¹Max-Planck Institut, Stuttgart, Germany; ²Helmholtz-Zentrum Berlin, Berlin, Germany; ³University of Tokyo, Tokyo, Japan; ⁴Argonne National Laboratory, Argonne, Illinois, USA

The recent discovery of multiferroicity associated with helical magnetic order in the insulating edge-sharing copper-oxide chain compounds LiCu₂O₂ and LiCuVO₄ has strongly stimulated the experimental and theoretical interest for these materials. The presence of defects generated by Li-Cu intersubstitution does however not allow distinguishing whether the substitutional disorder or the magnetic spiral is responsible for the ferroelectricity. We report our results on the NaCu₂O₂ compound which is isostructural to LiCu₂O₂ but free of substitutional disorder and twinning. Our study includes magnetic susceptibility measurements, resonant X-ray diffraction at the Cu L-absorption edge, polarization dependent X-ray absorption spectroscopy at the Cu L-edge and dielectric property measurements. Our measurements indicate the presence of a long-range magnetic spiral polarized within the bc plane below T_N = 12 K. The holes reside only on the Cu²⁺ sites in the copper-oxide chains and populate a d orbital polarized within the CuO₄ plaquettes. The dielectric measurements indicate the absence of electric polarization below T_N. We argue that these results support the scenario of substitutional disorder induced ferroelectricity in LiCu₂O₂.

3P081

Out-of-plane nesting-induced spin spiral in ultrathin Fe/Cu(001) films revealed by SX-ARPES

J Miyawaki,¹ A Chainani,¹ Y Takata,¹ M Mulazzi,¹ M Oura,¹ Y Senba,² H Ohashi,² S Shin^{1,3}

¹RIKEN SPring-8 Center, Sayo-gun, Hyogo, Japan; ²JASRI/SPring-8, Sayo-gun, Hyogo, Japan; ³Institute of Solid State Physics, The University of Tokyo, Kashiwa, Chiba, Japan

We investigate the origin of the spin spiral (SS) state in epitaxial ultrathin Fe films on Cu(001) using soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) [1]. Fe/Cu(001) films exhibit a SS in a thickness range of 5–11 monolayers (MLs), in contrast to the ferromagnetic bulk bcc Fe. We study the in-plane and out-of-plane Fermi surfaces (FSs) of the SS in 8 ML Fe/Cu(001) films at undulator beamline BL17SU of SPring-8 equipped with a grazing incidence geometry ($<5^\circ$) spectrometer. It was found that the SS originates from nested regions confined to out-of-plane FSs, which are drastically modified compared to in-plane FSs. The use of high energy soft X-rays ($h \sim 400\text{--}900$ eV) enables reciprocal space band mapping along k_z in the 4th and 5th Brillouin zones with high-precision. This plays a crucial role in identifying the associated real space compressive strain of $1.5 \pm 0.5\%$ along the c -axis. An autocorrelation analysis quantified the incommensurate ordering vector $\mathbf{q} = [2\pi/a](0, 0, \sim 0.86)$. These results are consistent with magneto-optic Kerr effect [2,3] and surface X-ray diffraction experiments [4] on the Fe/Cu(001) films, and suggest the importance of in-plane and out-of-plane FS mapping for ultrathin films.

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3P082

A practical approach correcting the saturation effect in XAS and XMCD spectra

JY Kim¹

¹Pohang Accelerator Laboratory & Department of Physics, POSTECH, Pohang, Kyungbuk, Republic of Korea

For decades, X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) in soft X-ray region have been important tools to probe the local state of transition metal ions and explore the microscopic origin of the magnetic properties of transition metals and rare earth compounds. The XAS spectra have been exclusively measured by an indirect method to detect the total electron yield (TEY) because of its simplicity and high sensitivity. Usually it is accepted that TEY is proportional to the absorption coefficient to a large extent. Nevertheless, the problem of saturation effect cannot be avoided in the quantitative analysis of XMCD spectra using TEY. This problem is caused by the large variation in X-ray penetration depth across the resonant absorption edges, and the relative intensities of prominent peaks in the TEY spectrum are reduced by the effect. Thus, the saturation correction is essential in a quantitative analysis, but it has been made in only a limited number of works, where a different set of samples grown on a special substrate as well as an additional set-up for the measurement of the other yields are required. In this work I suggest a new method to correct the saturation effect. Only the theoretical values of the X-ray penetration depth outside the region of resonant edges (before and after the edges) are used to calculate the theoretical electron yield and match it with the measured electron yield in the same unit, thereby eliminating the necessity of the independent transmission measurement. The reliability of this method is also confirmed by applying it to the XMCD spectra measured on an isotropic Fe polycrystal at two different angles before the sum rule analysis.

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3P083

X-ray absorption spectroscopy and X-ray magnetic circular dichroism study on the valence state and the spin structure of spinel $\text{Co}_{3-x}\text{Mn}_x\text{O}_4$ thin films

BG Park,¹ J Song,² JY Kim,¹ TY Koo¹

¹Pohang Accelerator Laboratory, Pohang, Gyeongbuk, Republic of Korea; ²Department of Physics, Chungnam National University, Daejeon, Republic of Korea

In AB_2O_4 spinel structures, A is 2+ cation at the tetrahedral (T_d) and B is 3+ one at the octahedral (O_h) site. If both A and B ions have local magnetic moment, a ferrimagnetic ordering is usually observed since the interaction between A and B ions is antiferromagnetic. However, an inversion between the each cation at A and B is very usual and the physical properties can be changed drastically by it. In this work, we analyzed the valence and spin state of $\text{Co}_{3-x}\text{Mn}_x\text{O}_4$ thin films grown on SrTiO_3 (100) single crystal substrates by pulsed laser deposition. The X-ray absorption spectroscopy (XAS) spectra at Co K -edge and $L_{2,3}$ -edges show that Co ions are mixed valent with the valence of 2+ and 3+. A quantitative analysis of the XAS spectra indicates that Co^{2+} ions are in T_d sites and Co^{3+} ions are in O_h sites. The X-ray magnetic circular dichroism (XMCD) at Co $L_{2,3}$ -edges also shows that Co^{2+} ions in T_d sites are in high spin state ($S=3/2$), but Co^{3+} ions in O_h sites are in low spin states ($S=0$). The identical measurement on Mn ions also shows a consistent result that the Mn ions are mixed-valent as well and occupies O_h sites with high spin state.

This work was supported by National Research Foundation of Korea Grant funded by the Korean Government (Grant No. 2009-0088969 and KRF-2008-314-C00249).

3P084

X-ray magnetic circular dichroism study of room-temperature ferromagnetism in Fe-doped TiO_2

E Sakai,¹ K Amemiya,³ A Chikamatsu,¹ Y Hirose,^{1,2} T Shimada,^{1,2} T Hasegawa^{1,2}

¹The University of Tokyo, Tokyo, Japan; ²KAST, Kawasaki, Kanagawa, Japan; ³KEK-PF, Tsukuba, Ibaraki, Japan

We have performed X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) measurements of both paramagnetic and ferromagnetic $\text{Ti}_{1-x}\text{Fe}_x\text{O}_2$ thin films under a relatively weak field of 0.1 T. The Fe L_3 and L_2 edge XAS spectra showed two characteristic peaks at 707 and 709 eV, respectively, which were attributable to Fe^{2+} and Fe^{3+} states. On the basis of a comparison of the intensity ratio of these two peaks with those of the Fe^{2+} and Fe^{3+} reference materials, we concluded that the Fe ions in our samples are in mixed valence states and that the $\text{Fe}^{2+}/\text{Fe}^{3+}$ ratio is a decreasing function of partial oxygen pressure during deposition. XMCD signals were observed only for the Fe^{2+} peaks of ferromagnetic samples, indicating that the room-temperature ferromagnetism in $\text{Ti}_{1-x}\text{Fe}_x\text{O}_2$ is an intrinsic property, where the ferromagnetic interaction between Fe^{2+} local spins plays an essential role. This result suggests that the configuration of iron ions and oxygen vacancies in $\text{Ti}_{1-x}\text{Fe}_x\text{O}_2$ affect the magnetic properties.

3P085

Evidence for Ti 3d carrier-induced ferromagnetism in anatase Co:TiO₂ thin films

T Ohtsuki,¹ A Chainani,¹ R Eguchi,^{1,2} M Matsunami,^{1,2} Y Takata,¹ M Oura,¹ Y Senba,³ H Ohashi,³ Y Nishino,¹ K Tamasaku,¹ M Yabashi,³ T Ishikawa,^{1,3} T Hasegawa,^{4,5} S Shin^{1,2}

¹RIKEN SPring-8 Center, Sayo-cho, Sayo-gun, Hyogo, Japan; ²Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba, Japan; ³JASRI/SPring-8, Sayo-cho, Sayo-gun, Hyogo, Japan; ⁴Department of Chemistry, The University of Tokyo, Bunkyo-ku, Tokyo, Japan; ⁵Kanagawa Academy of Science and Technology (KAST), Takatsu-ku, Kawasaki, Japan

Diluted magnetic semiconductors (DMSs) are compound semiconductors containing a small amount of a magnetic element. They have attracted much attention because DMSs utilize spin and charge degrees of freedom, and are considered strong candidates for spintronic materials. From previous studies, Co-doped TiO_2 [Co:TiO₂] is known to show ferromagnetism far above room temperature. However, its origin and mechanism have not been fully understood. Therefore, we felt it important to study the electronic structure of Co:TiO₂. In this study, we fabricated anatase Co:TiO₂ thin films on SrTiO₃(100) substrate by the pulsed laser deposition (PLD) method. In order to understand the electronic structure of anatase Co:TiO₂, soft and hard X-ray photoemission spectroscopy (SX-PES and HAXPES, respectively) have been measured. Furthermore, X-ray absorption spectroscopy (XAS) and high-sensitivity resonant photoemission spectroscopy (RPES) have been carried out in soft X-ray region. The measurements were performed at undulator beamline BL17SU (for SX-PES) and BL29XU (for HAXPES) of SPring-8. The results indicate that anatase Co:TiO₂ thin films are thought to exhibit intrinsic ferromagnetism due to a carrier-induced mechanism involving Ti 3d states.

3P086

Nano-roughness in gold revealed from X-ray signature

JL Glover,¹ CT Chantler¹

¹School of Physics, University of Melbourne, Parkville, Victoria, Australia

We present a new method for investigating roughness for surface structure and internal inhomogeneity down to the nano-scale for thin, nano-structured and opaque materials. The method uses careful measurements of the X-ray mass-attenuation coefficient and is applied to measure the magnitude of the roughness of gold foils. The technique is unique, providing insight into both surface and internal roughness. We show that moments of the distribution function of surface and internal structure can be investigated using this method, and discuss observable signatures. The approach is non-destructive and very sensitive as a local in situ measurement and as a diagnostic for accurate characterisation.

[1] J. L. Glover et al, Phys Lett A373 (2009) 1177-1180

3P087

Soft X-ray photoemission study of thermoelectric alloys $\text{Fe}_{2-x}\text{V}_y\text{Ir}_{1-x}\text{Ti}_y\text{Al}$ and $\text{Fe}_{2-x}\text{V}_{1+x-y}\text{Ti}_y\text{Al}$

K Soda,¹ S Harada,¹ M Kato,¹ S Yagi,¹ M Inukai,² H Miyazaki,³ Y Sandaiji,⁴ S Tanaka,⁴ Y Tamada,⁴ T Sugiura,⁴ Y Nishino⁴

¹Department of Quantum Engineering, Graduate School of Engineering, Nagoya University, Nagoya, Japan; ²Venture Business Laboratory, Nagoya University, Nagoya, Japan;

³Institute for Molecular Science, Okazaki, Japan; ⁴Department of Frontier Materials, Graduate School of Engineering, Nagoya Institute of Technology, Nagoya, Japan

The valence-band and core-level photoemission spectra of the n-type thermoelectric Heusler(L₂₁)-type alloys $\text{Fe}_{2-x}\text{V}_y\text{Ir}_{1-x}\text{Ti}_y\text{Al}$ and p-type ones $\text{Fe}_{2-x}\text{V}_{1+x-y}\text{Ti}_y\text{Al}$ have been investigated in order to clarify the origin of the remarkable enhancement of their thermoelectric power in comparison with the stoichiometric ($x = 0$) alloys. For the n-type alloys, a shoulder structure with small intensity is recognized around the Fermi level E_F , indicative of the pseudogap predicted by a band structure calculation, and the intense d band with a steep edge just below E_F is found for the p-type alloys. These spectral features are consistent with a theoretical dependence of the thermoelectric power on the electronic density of states. Whereas the energy position of E_F is moderately shifted in a rigid-band-like manner on the partial substitution y of Ir and Ti, the valence-band spectra near E_F show a non-rigid-band-like behavior for the off-stoichiometric concentration change x . Observed satellite structures in the V $2p$ core-level spectra for the off-stoichiometric alloys with $x > 0$ suggest the V anti-site defect, *i.e.* the excess V occupying at the Fe site of the Heusler-type structure. The non-rigid-band-like change is ascribed to the Fe or V anti-site defect formation in the off-stoichiometric alloys and the rigid-band-like shift to the common band formation with the Ir $5d$ or Ti $3d$ states incorporated into the main Fe-V $3d$ bands on the partial substitution, respectively. The remarkable enhancement of the thermoelectric power in those Heusler-type alloys can be successfully explained in terms of the observed changes in the valence-band electronic structure near E_F .

3P088

Electronic structures of LaB_6 and CeB_6 single crystals: a spectroscopic investigation of the $4d$ - $4f$ transitions

L Liu,¹ YM Yiu,¹ TK Sham¹

¹Department of Chemistry, University of Western Ontario, London, Ontario, Canada

X-ray absorption near-edge structures (XANES) of rare earth hexaboride (LaB_6 and CeB_6) single crystals have been studied at the La and Ce $N_{5,4}$ -edges. The spectra are composed of a group of sharp pre-edge resonances and a broad giant resonance above the edge, which are due to transitions from $4d^{10}4f^0$ to $4d^9 4f^{n+1}$. The difference in the occupancy of $4f$ electrons between ground state La ($4d^{10}4f^0$) and Ce ($4d^{10}4f^1$) causes significantly differences in $N_{5,4}$ -edge XANES both below and above the edge. LaB_6 shows two sharp pre-edge peaks at 97.4 eV and 101.3 eV and a broad resonance at 118.2 eV while CeB_6 shows ten well-resolved pre-edge peaks at energy between 100-112 eV and two post-edge peaks at 121.7 eV and 125.2 eV, respectively. Theoretical simulations using the FEFF9 and WIEN2k code have been conducted to compare with the experiment and previous atomic calculations. The results and their implications are discussed.

Research at UWO is supported by NSERC, CFI, OIT and CRC. Synchrotron experiments were conducted at the Canadian Light Source, which is supported by NSERC, NRC, CIHR and the University of Saskatchewan.

3P089

Change of Co distribution accompanied with degradation in membrane electrolyte assembly with Pt-Co cathode catalysts for PEFC

M Kobayashi,^{1,2,3} S Hidaï,^{1,4} H Niwa,¹ Y Harada,^{1,2,3} M Oshima,^{1,2} Y Horikawa,³ T Tokushima,³ S Shin,^{3,5} H Ofuchi,⁶ Y Nakamori,⁴ T Aoki⁴

¹Department of Applied Chemistry, School of Engineering, University of Tokyo, Bunkyo-ku, Tokyo, Japan; ²Synchrotron Radiation Research Organization, The University of Tokyo, Sayo-cho, Sayo-gun, Hyogo, Japan; ³RIKEN/SPring-8, Sayo-cho, Sayo-gun, Hyogo, Japan; ⁴Toshiba Fuel Cell Power Systems Corporation, Kawasaki-ku, Kawasaki-Shi, Kanagawa, Japan; ⁵Institute for Solid State Physics, University of Tokyo, Kashiwanoha, Kashiwa, Chiba, Japan; ⁶Japan Synchrotron Radiation Research Institute (JASRI), Sayo-cho, Sayo-gun, Hyogo, Japan

Polymer electrolyte fuel cells (PEFCs) have attracted much attention as energy conversion devices because the main product generated by electrochemical reactions of PEFC is water. PEFCs have a cell structure called a membrane electrode assembly (MEA), in which a proton exchange membrane is sandwiched between the cathode and the anode. In order to improve the performance of PEFC, it is important to understand degradation of MEA after the electrochemical operation. In this work, the electronic structures of a Pt-Co cathode catalyst and a Pt-Ru anode catalyst in MEA have been investigated using X-ray absorption fine structure (XAFS) spectroscopy and soft X-ray absorption spectroscopy (XAS). XAS microscopy has been performed with a $1.0 \mu\text{m}$ focused beam in the vertical direction on an oblique section of the samples before and after a degradation test. The observations provide us with fundamental understanding on the changes of element-specific distribution and chemical states in MEA after the electrochemical reaction.

3P090

Application of fluorescence-yield XAS to the studies of organic thin-film devices: observation of hidden electronic states and its field effect

HS Kato,¹ H Yamane,² N Kosugi,² M Kawai^{1,3}

¹Advanced Science Institute, RIKEN, Wako, Saitama, Japan; ²Institute for Molecular Science (IMS), Okazaki, Aichi, Japan; ³Department of Advanced Materials Science, University of Tokyo, Kashiwa, Chiba, Japan

The electronic states of organic thin film devices have been studied using X-ray absorption spectroscopy (XAS) in the bulk-sensitive fluorescence yield (FY) mode. Since the soft X-ray has a long penetration depth of about 100 nm, it is able to directly observe hidden electronic states in the films even beneath metal electrodes [1]. In addition, because the X-rays are not disturbed by applied electric field, different from emitted electrons, FY-XAS enables us to study the electronic states of organic thin film devices under operating condition [2]. For the investigation of organic thin film transistors, the well-oriented pentacene and oligothiophene thin films (a few 10 nm thick) on the SiO₂-precovered Si substrates with top-contact Au electrodes (25 nm thick) were prepared. First, we confirmed that, by the incident angle dependence of the C K-edge FY-XAS spectra, the Au electrode deposition has not significantly perturbed the molecular orientation in the thin films. Then, the gate bias dependence of the FY-XAS spectra of the thin films was attempted and successfully detected the spectral changes which show obviously different shape from original spectra. The origin of the spectral change is considered to be some distortion of molecular orbital depending on the applied bias, and thus the modified spectra should inform us about a distribution of local electric field in the films [2].

[1] H.S. Kato, *et al.*, J. Electron Spectrosc. Relat. Phenom. 174 (2009) 93.

[2] H.S. Kato, H. Yamane, N. Kosugi, M. Kawai, (to be published).

3P091

Overview of the GALAXIES beamline at the SOLEIL synchrotron: inelastic X-ray scattering and hard X-ray photoemission spectroscopy.

JP Rueff^{1,2}

¹Synchrotron SOLEIL, Gif-sur-Yvette, France; ²Laboratoire de Chimie Physique - Matière et Rayonnement, UPMC - CNRS, Paris, France

The GALAXIES beamline at the SOLEIL synchrotron is dedicated to novel X-ray spectroscopic techniques using hard X-rays, namely inelastic X-ray scattering (IXS) and hard X-ray photoemission spectroscopy (HAXPES). IXS is a selective probe of the electronic structure and collective dynamics of materials. Owing to its all-photon aspect, it has bulk sensitivity and is well suited to samples in difficult environments such as in a high pressure cell. On the other hand, HAXPES clearly extends the capacities of photoemission, a widely utilized probe for chemical analysis and study of the electronic properties, towards high kinetic energy and bulk sensitivity. These two techniques thus offer rich and complementary information which make the beamline well adapted to investigating complex materials in the solid state, among which strongly correlated materials, heavy fermions and actinides compounds, and diluted phases (liquid, gas) from the point of view of the electronic properties. The beamline optics has been optimized for best performances in terms of photon flux, micro-focalization, and resolving power in the 2.3-12 keV energy range. We will present the main beamline characteristics, and potential applications. The GALAXIES beamline will offer ample opportunities for a vast community of users ranging from condensed matter physics to chemistry, Earth science or atomic / molecular physics.

3P092

Zone plate based soft X-ray lithography

AFG Leontowich,¹ AP Hitchcock¹

¹McMaster University, Department of Chemistry, Hamilton, Ontario, Canada

We use X-rays focused to ~30 nm in scanning transmission X-ray microscopes (STXM) to pattern polymer thin films in a manner analogous to pattern generation with a focused electron beam in e-beam lithography systems. Under optimized conditions developed lines <50 nm wide have been produced in poly(methylmethacrylate). The photon energy tunability of the STXM can be used for chemically selective patterning of polymers consisting of 2 or 3 layers of different polymer types – e.g. PMMA, polystyrene and polyethylcarbonate [1,2]. When high doses are administered radiation damage is observed well outside the position of the beam on the sample. This can extend more than 1 μm beyond the well defined exposure area. A multi-technique approach combining near edge X-ray absorption fine structure spectromicroscopy, chemical development, atomic force microscopy and scanning electron microscopy is being used to investigate processes of radiation damage and damage migration in polymers. The ultimate outcome is expected to be a much improved understanding of radiation chemistry and physics of resist materials.

Work performed at Advanced Light Source beamline 5.3.2 (Berkeley, California, U.S.A.) supported by BES-DoE.

[1] Wang, J.; Stöver, H. D. H.; Hitchcock, A. P.; Tylliszczak, T. J. Synchrotron Rad. 2007, 14, 181.

[2] Wang, J.; Stöver, H. D. H.; Hitchcock, A. P. J. Phys. Chem. C 2007, 111, 16330.

3P093

Silicon drift detector applications in soft X-ray absorption spectroscopyTZ Regier,¹ RIR Blyth,¹ D Chevrier,¹ D Beaugregard,¹ A Achkar,² H Wadati,³ DG Hawthorn²¹Canadian Light Source, Inc., Saskatoon, Saskatchewan, Canada; ²University of Waterloo, Waterloo, Ontario, Canada; ³University of British Columbia, Vancouver, British Columbia, Canada

We report on the operation of a Silicon Drift Detector (SDD) installed on the endstation of the SGM (11ID-1) beamline at the Canadian Light Source (CLS). This facilitates the collection of a complete X-ray Fluorescence (XRF) spectrum for each excitation energy in a Near Edge X-ray Absorption Fine Structure (NEXAFS) measurement. The new capability allows for the easy identification of 2nd order and scattering contributions to the total fluorescence yield. It also allows for the acquisition of the Partial Fluorescence Yield (PFY) from both the on and off resonance elements in the sample. Using this capability, we demonstrate exciting results that show that the Inverse PFY (IPFY) from an off-resonant element can be used as a self absorption free probe of the bulk X-ray absorption cross section. Examples of these new applications will be presented and discussed for several different sample systems.

3P094

Resonant photoemission and X-ray absorption of organic Europium complexesJ Thompson,¹ V Arima,² L Carbone,² T Regier,¹ L Zuin,¹ YF Hu,¹ TK Sham,⁴ BP Doyle,³ RIR Blyth¹¹Canadian Light Source, Saskatoon, Saskatchewan, Canada; ²National Nanotech Laboratory of CNR-INFN, Lecce, Puglia, Italy; ³TASC-INFN Laboratory, Trieste, Italy; ⁴Department of Chemistry, University of Western Ontario, London, Ontario, Canada

Resonant photoemission and X-ray absorption (XAS) measurements at the 3d and 4d edges of Eu are investigated as possible probes of the valence state of Eu in organic complexes. Deliberate conversion of Eu³⁺ to Eu²⁺, by radiation exposure allowed for the distinction of the 3+ and 2+ states of Eu in the 3d absorption spectra. XAS measurements are found to be relatively insensitive to the presence of small amounts of 2+ in a nominally 3+ Eu complex. 3d resonant photoemission, in contrast, is found to be a highly promising probe.

Resonant photoemission was then used to investigate the presence of Eu²⁺ in wet-processed films of nominally 3+ commercial red-emitting Eu complexes, in order to replicate simple device processing conditions. Significant amounts of Eu²⁺ were found, suggesting that even wet deposition from solvents may well affect the chemistry and therefore the ultimate performance of these molecules within a device such as an OLED.

3P095

Resonant Auger at the Cu L₃-edge of Cu₃Au: implications for resonant inelastic X-ray scattering (RIXS) and core-hole decay dynamicsRIR Blyth,¹ TZ Regier,¹ TK Sham²¹Canadian Light Source, Saskatoon, Saskatchewan, Canada; ²Dept. of Chemistry, University of Western Ontario, London, Ontario, Canada

Resonant Auger is a competing phenomenon to Resonant Inelastic X-ray Scattering (RIXS) of the fluorescence channel. In Resonant Auger the absorption of the photon and the decay of the core-hole have to be viewed as a concerted event, and, in contrast to the normal Auger process, the resonant Auger spectrum exhibits energy dispersion. This is analogous to the constant energy transfer in RIXS, and arises when the core hole decays before its relaxation is completed. This results in the suppression of lifetime broadening in the Auger lines at resonance. Experimentally, however, the conditions required to observe these effects are stringent, especially for narrow core-hole linewidth. High resolution is required such that the overall experimental resolution is smaller than the lifetime broadening of the core hole. We report here Cu L-edge resonant Auger Spectroscopy of Cu₃Au obtained at the SGM beamline at the Canadian Light Source. Photon energies were selected from several eV below the Cu L₃-edge to above the Cu L₂ and L₁ edges. Auger spectra were recorded with photon energy increments small as 0.1 eV. The dispersion is clearly seen in the pre-edge region. The dispersion diminishes quickly above resonance and the Auger energy approaches a constant. The L₂- and L₁-edge excitations show more complex features as Coster-Kronig transitions turn on at these edges. Suppression of the Auger linewidth is immediately apparent from a comparison of spectra on and above resonance.

3P096

The nitrogen K shell absorption spectrum of trimethylsilyl azide

R Cavell,¹ A Jürgensen¹

¹Dept of Chemistry, University of Alberta, Edmonton, AB, Canada

Trimethylsilyl azide is a well known, very stable, molecular azide which is widely used as a reagent for organic and organometallic reactions forming imines by means of elimination of molecular nitrogen. In contrast the similarly constituted hydrazoic acid is a treacherous explosive. The silylated form thus provides a safe analog for spectroscopic evaluation of the X-N=N=N molecular structure. The N₃ portion of the molecule is well known to be linear and the X substituent is bent away from the N₃ axis. The structure renders each nitrogen unique and distinct. The gas phase spectrum in the nitrogen K shell absorption region, measured with the Canadian Spherical Grating monochromator beamline, consisting of two distinct peaks was interpreted with the assistance of the GSCF3 code (following optimization of the molecular geometry with GAMESS US) which identified MO transition energies and oscillator strengths. The lower energy peak at 402 eV is assigned to a combination of transitions from the terminal nitrogen N_A and the substituted nitrogen N_C, both of which bear net negative charge. The central nitrogen, N_B, has a positive charge and transitions arising there from are attributed to the higher energy peak at 406 eV. Additional peaks are assigned to transitions to the delocalized π* MO structure of the molecule, again aided by the calculations. [We thank N Kosugi for access to the GSCF3 code.]

3P097

Investigation of cluster structure of liquid metals

AV Murin,¹ IN Shabanova,¹ AV Kholzakov¹

¹Physicotechnical Institute of the Ural Division of the Russian Academy of Sciences, Izhevsk, Russian Federation

The information about the structure of metal melts is key information for controlling the synthesis of nanostructures having some definite shapes. It is known that the liquid system structure is inherited at cooling. In the present work, the investigation of the nanoscale cluster structure of d-metals and their systems in the liquid state was carried out. The comparative study was conducted for the theoretical models of the structure of liquids of d-metals (Ni, Cu and Au) made by the method of classical molecular dynamics. The many-body semiempirical potentials of the embedded atom method were used. The structures of liquid metals were used as input data for: [a] the calculation of the radial distribution function (RDF); [b] the conduction of calculations of the electronic structure; [c] the analysis of the cluster structure based on the metrics which describe quantitatively the nearest surrounding of atoms. In addition, the X-ray photoelectron investigation of the electronic structure of d-metals and their systems in the liquid state was carried out. The approach of atoms in the liquid state leads to the strong redistribution of the electron density between the atoms, and the strong hybridization of d- with p-electrons is observed depending on the localization of d-electrons in the metals under study, which determines the shape of valence bands and the curve of the total density of electron states (DOS). As a result, clusters with strong interatomic bonds are formed. Good agreement of the calculated and experimental RDFs and also of the calculated DOS and XPS spectra allows to draw a conclusion about the adequacy of the results of modeling of the atomic structure and the following cluster analysis. The shape of the nano-clusters and the cluster composition of the liquids of the d-metals' systems depending on filling their d-shell are discussed.

3P098

Solution-structure analysis of saccharides by synchrotron-radiation vacuum-ultraviolet circular dichroism spectroscopy

K Matsuo,¹ K Gekko,^{1,2} T Fukuyama,² H Namatame,¹ M Taniguchi^{1,2}

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan

Saccharides take complicated equilibrium conformations in aqueous solution which are closely related to their biological functions. A vacuum-ultraviolet circular dichroism (VUVCD) spectroscopy using a synchrotron radiation is useful for analyzing these solution structures of saccharides because this method allows us to detect the high-energy chromophores such as hydroxyl and acetal groups in the VUV region below 190 nm. In the present study, we report the VUVCD spectra of various saccharides down to 160 nm in aqueous solution and discuss their solution structures based on the theoretical analysis. The VUVCD spectra of most monosaccharides showed a positive peak with some shoulders at around 170 nm mainly due to the n-π* transition of ring oxygen atom. These spectra sensitively reflected the structural characteristics such as α- and β-anomers, axial and equatorial hydroxyl groups, and trans (T) and gauche (G) configurations of hydroxymethyl group. The contributions of these configurations were estimated by the deconvolution analysis of the VUVCD spectra and confirmed by the VUVCD spectra of α-GG, α-GT, β-GG, and β-GT conformers of methyl α- and β-D-glucopyranosides, which were reasonably calculated by the time-dependent density functional theory taking into consideration three water molecules around them. These results demonstrate that the synchrotron-radiation VUVCD spectroscopy combined with theoretical analysis is powerful for understanding the solution structures of saccharides.

3P100

Pressure-induced electronic and structural transformations in multiferroic BiMnO₃ probed by lifetime-broadening-suppressed X-ray absorption spectroscopy and X-ray emission spectroscopy

JM Chen,¹ JM Lee,¹ SC Haw,¹ TL Chou,¹ SA Chen,¹ KT Lu,¹ E Huang,² YC Liang,¹ SW Chen,¹ JF Lee,¹ N Hiraoka,¹ H Ishii,¹ KD Tsuei,¹ TJ Yang³

¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Center for General Education, Chung Chou Institute of Technology, Changhua County, Taiwan; ³Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan

Pressure-induced electronic and structural transformations in multiferroic BiMnO₃ were probed by lifetime-broadening-suppressed X-ray absorption spectroscopy (XAS) and X-ray emission spectroscopy. The Mn *K*-edge high-resolution XAS spectra and Mn *Kβ* emission spectra of polycrystalline BiMnO₃ were collected at various pressures in the range 0.5 – 43 GPa. The Mn *K*-edge absorption spectra were obtained in the partial fluorescence yield, with the spectrometer energy fixed at the maximum of the Mn *Kβ*_{1,3} line. The Mn *K*-edge XAS spectra of BiMnO₃ show a dramatic change for pressure below 2 GPa, implying that a phase transition occurs between about 1.5 and 5.5 GPa. In contrast, the Mn *K*-edge XAS spectra exhibit slight modifications in the pressure range 2 - 43 GPa, indicating that the local atomic manganese environment is not drastically changed under external hydrostatic pressure > 2 GPa. There is no appreciable change in the Mn *Kβ* emission spectra for pressure in the range 2 – 20 GPa. The *Kβ*' intensity is notably reduced for external pressure larger than 30 GPa, indicating a significant loss of magnetic moment in BiMnO₃. Based on present high-pressure XAS and X-ray emission studies, we did not observe any phase transition of BiMnO₃ for pressure > 8 GPa.

3P101

Behaviour of sodium halide ions in microscopic interfaces of mixed solvents observed via X-ray absorption spectroscopy

MH Rittmann-Frank,^{1,2} KM Lange,¹ U Bergmann,³ KF Hodeck,¹ R Könnecke,¹ U Schade,¹ N Ottosson,⁴ W Pokapanich,⁴ M Chergui,²
MW Linscheid,³ EF Aziz¹

¹Helmholtz Zentrum Berlin für Materialien und Energie (BESSYII), Berlin, Germany; ²Ecole Polytechnique Fédérale de Lausanne, Lausanne-Dorigny, Switzerland; ³Humboldt University in Berlin, Berlin, Germany; ⁴Uppsala University, Uppsala, Sweden

We present a soft X-ray absorption study on sodium ions with different counter ions that sheds light on the ion pairing process in pure, as well as in mixed solvents of different polarity (i.e. water, methanol, ethanol, propanol). Although water and alcohol were shown to be unmixable on microscopic scales, our study reveals that the addition of sodium ions to a mixture of water and alcohol facilitates a shared solvation of the ions by the solutes. Our study reveals also a solvent-selective photochemical process linked to iodine counter ions which takes place in an alcohol solvent, but not in water. We show in our study that, adding water to the alcohol inhibits the photochemical process, due to the formation of sodium-iodide complexes at the solvent interface. Our study reports for the first time the behaviour of ions at such mixed-solvent interfaces on microscopic scales.

WEDNESDAY PROGRAM

4PL Ultrafast science

Chair: Paul Corkum

8:30 - 10:10

LIFE SCIENCES INSTITUTE 2

4PL1 **Ferenc Krausz** (plenary)

8:30 Attosecond physics

4PL2 **David Villeneuve** (invited)

9:10 Using high harmonic spectroscopy to learn about molecular structure and dynamics

4PL3 **Hermann Dürr** (invited)

9:40 Femtosecond spin-orbit excitations in ferromagnets

EXCURSIONS

WHISTLER Buses leave UBC at 10:45

Return times (board bus at Whistler): EARLY 18:00, LATE 20:30

Please sign up for your return time at the registration desk.

DEEP COVE Buses leave UBC at 10:45

Buses leave Deep Cove at 16:00

TRIUMF Tours will start at 11:30, 13:30, and 15:30 at the entrance to TRIUMF and will last approximately 90 minutes.

Delegates must choose their preferred tour time at the registration desk by the end of Tuesday, July 13. Information about transport to the TRIUMF facility (which is about 2 km from LSI) will be provided at the registration desk. If you intend to walk, please allow one half-hour to do so.

4PL1

Attosecond physics

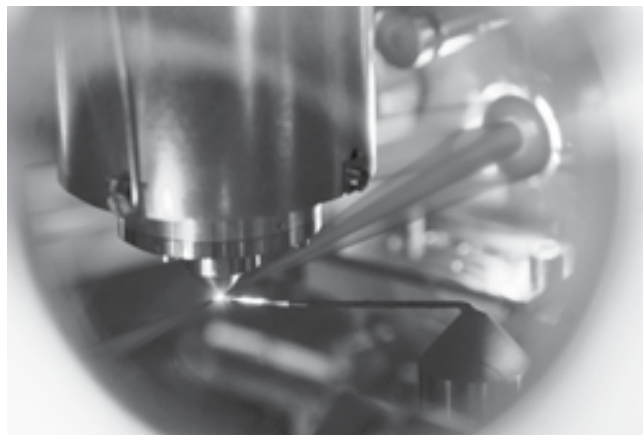
Ferenc Krausz^{1,2,3}

¹ Max-Planck-Institut für Quantenoptik, Garching, Germany. ² Ludwig-Maximilians-Universität München, München, Germany
³ www.attoworld.de

Electronic motion is a key process in a wide range of modern technologies, including micro- to nano-electronics, photovoltaics, bioinformatics, molecular biology, and medical as well as information technologies. The atomic-scale motion of electrons typically unfolds within tens to thousands of attoseconds (1 attosecond [as] = 10^{-18} s). Recent advances in laser science have opened the door to watching and controlling these hitherto inaccessible microscopic dynamics [1]-[13]. Key tools include waveform-controlled few-cycle laser light and attosecond extreme ultraviolet pulses. They permit control of atomic-scale electric currents just as microwave fields control currents in nanometer-scale semiconductor chips. By analogy to microwave electronics, we have dubbed this new technology “lightwave electronics” [10,12]. Lightwave electronics provides – for the first time – real-time access to the motion of electrons on atomic and sub-atomic scales. Insight into and control over microscopic electron motion are likely to be important for developing brilliant sources of X-rays, understanding molecular processes relevant to the curing effects of drugs, the transport of bioinformation, or the damage and repair mechanisms of DNA, at the most fundamental level, where the borders between physics, chemistry and biology disappear. Once implemented in condensed matter, the new technology will be instrumental in advancing electronics and electron-based information technologies to their ultimate speed: from microwave towards lightwave frequencies.

[1] M. Hentschel et al., Nature 414, 509 [2001]; [2] R. Kienberger et al., Science 291, 1923 [2002]; [3] A. Baltuska et al., Nature 421, 611 [2003]; [4] R. Kienberger et al., Nature 427, 817 [2004]; [5] E. Goulielmakis et al., Science 305, 1267 [2004]; [6] M. Drescher et al., Nature 419, 803 [2002]. [7] M. Uiberacker et al., Nature 446, 627 [2007]; [8] M. Kling et al., Science 312, 246 [2006]; [9] A. Cavalieri et al., Nature 449, 1029 [2007]; [10] E. Goulielmakis et al., Science 317, 769 [2007]; [11] E. Goulielmakis et al., Science 320, 1614 [2008]. [12] F. Krausz, M. Ivanov, “Attosecond Physics,” Rev. Mod. Phys. 81, 163 [2009]. [13] M. Fuchs et al., Nature Phys. 5, 826 [2009].

Attosecond pulses of extreme ultraviolet light are focused by a mirror (right) on a jet of neon atoms as an infrared beam strikes the atoms, allowing real-time observation of the motion of electrons in Ne and measurement of the duration of the attosecond pulse. (Photo: Thorsten Naeser; image editing: Christian Hackenberger)



Ferenc Krausz was awarded his M.S. in Electrical Engineering at Budapest University of Technology in 1985, his Ph. D. in Quantum Electronics at Vienna University of Technology in 1991,

and his “Habilitation” degree in the same field at the same university in 1993. He joined the Department of Electrical Engineering as Associate Professor in 1998 and became Full Professor in the same department in 1999. In 2003 he was appointed as Director of Max Planck Institute of Quantum Optics in Garching, Germany, and since October 2004 he has also been Professor of Physics and Chair of Experimental

Physics at Ludwig Maximilian's University of Munich. His research has included the examination of nonlinear light-matter interactions, ultrashort light pulse generation from the infrared to the X-ray spectral range, and studies of ultrafast microscopic processes. By using chirped multilayer mirrors, his group has made intense light pulses comprising merely a few wave cycles available for a wide range of applications and utilized them for pushing the frontiers of ultrafast science into the attosecond regime. His most recent research focuses on attosecond physics: the control and real-time observation of the atomic-scale motion of electrons. Prof. Krausz co-founded Femtolasers GmbH, a Vienna-based company specializing in cutting-edge femtosecond laser sources.

4PL2 (invited)**Using high harmonic spectroscopy to learn about molecular structure and dynamics**DM Villeneuve¹¹National Research Council, Ottawa ON, Canada

High harmonic generation in atoms and molecules can be viewed as a time-reversed photoionization process. An electron is removed from the parent by an intense femtosecond laser field. The electron is then driven back to the parent ion by the same field within one optical cycle. The electron can recombine back to the ground state, and thereby emit an XUV photon. The recombination dipole moments are very similar to photoionization dipole moments, and contain information about the electronic structure of the parent molecule. High harmonic spectroscopy has several advantages over photoionization, such as the highly parallel measurement at many photon energies simultaneously, the ability to measure polarization and phase of the photons, the high time resolution, and the ability to align the molecules in space. We apply high harmonic spectroscopy to study the unimolecular dissociation of the bromine molecule. We show that the strong emission from unexcited molecules acts as a local oscillator in a homodyne detection scheme, and permits the measurement of both amplitude and phase of the excited state emission. Using a transient grating excitation geometry in bromine, we can follow the dissociating molecules along the reaction coordinate. Because high harmonic spectroscopy is sensitive to the electronic state of a molecule, this technique shows promise to observe changes in electronic structure during a chemical reaction, for example at conical intersections.

4PL3 (invited)**Femtosecond spin-orbit excitations in ferromagnets**H Dürr¹¹PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, United States

Polarized soft X-rays have been used over the past 20 years to obtain fascinating new insights into nanoscale magnetism. The separation of spin and orbital magnetic moments, for instance, enabled detailed insights into the interplay of exchange and spin-orbit interactions at the atomic level. The now available polarized soft X-ray pulses with only 100 fs duration allow us to observe the magnetic interactions at work in real time. The ultimate goal of such studies is to understand how spins may be manipulated by ultrashort magnetic field, spin polarized current or light pulses. In this talk I will focus on fs laser induced spin-orbit dynamics in 3d transition metals, 4f systems and their alloys. Using fs X-ray pulses from the BESSY II femtoslicing facility I will show how fs excitation of the electronic system modifies the spin-orbit interaction enabling ultrafast angular momentum transfer between spin, orbital and lattice degrees of freedom. An outlook will be given on how X-ray free electron laser radiation will revolutionize this field.

THURSDAY PROGRAM

5PL Coherent Imaging
Chair: Wolfgang Eberhardt

9:00 - 10:10

LIFE SCIENCES INSTITUTE 2

5PL1 Henry Chapman (plenary)

9:00 Coherent X-ray diffraction imaging at the LCLS

5PL2 Akiyoshi Hishikawa (invited)

9:40 Visualizing ultrafast chemical reactions by intense ultrashort laser pulses

Coffee

10:10 - 10:40

5A Fourth generation sources & science

Chair: John Bozek 10:40 - 12:30

LIFE SCIENCES INSTITUTE 2

5A1 Tsutomu Shintake (invited)

10:40 Status of the SCSS X-ray Free Electron Laser XFEL/SPring-8 Project in Japan

5A2 Serguei Molodtsov

11:10 The European XFEL project: status and research applications

5A3 Gilad Marcus

11:30 keV high harmonic and K-shell excitation using a 2-cycle IR (2.1 micron) radiation source

5A4 Dimitrios Charalambidis

11:50 News and views from the attosecond generation, characterization and applications frontier

5A5 Daniel Rolles

12:10 Time-resolved photoelectron diffraction on laser-aligned molecules

5B Magnetism resolved in time and space

Chair: Ziyi Wu 10:40 - 12:30

FOREST SCIENCES 1005

5B1 Peter Fischer (invited)

10:40 Magnetic soft X-ray microscopy: achievements and future opportunities to image fast spin dynamics in nanomagnetism

5B2 Benjamin Balke

11:10 Depth-resolved magnetism and valence band densities of states for the magnetic tunnel junction interface Fe/MgO via standing-wave excited photoelectron emission and magnetic circular dichroism

5B3 Der Hsin Wei

11:30 Responses of an ultrathin cobalt film in contact with an organic pentacene layer

5B4 Stephen Kevan

11:50 Slow dynamics in Au/Co/Au thin films near the spin-reorientation transition

5B5 Tsuneaki Miyahara

12:10 MCD Study on Ce@C₈₂ and Ce₂@C₈₀ in the soft X-ray region

Lunch

12:30 - 14:00

5C Atoms & Molecules (2)

Chair: John Bozek 14:00 - 16:10

LIFE SCIENCES INSTITUTE 2

5C1 Nobuhiro Kosugi (invited)

14:00 Molecular inner-shell spectra of weakly bonding and interacting systems

5C2 Joakim Laksman

14:30 Dynamics of terminal atom migration and dissociation in small core-excited molecules probed by multiple ion momentum imaging

5C3 Alexandre Lago

14:50 Photodissociation dynamics of the chloroform molecule excited in the vicinity of the Cl 1s edge

5C4 Ayako Yamada

15:10 Sequential multi-photon multiple-ionization of molecules by EUV free-electron laser at SPring-8

5C5 Giovanni Stefani

15:30 Electronic properties of thin magnetic films probed by Auger photoelectron coincidence spectroscopy (APECS)

5C6 Raimund Feifel

15:50 Multi-electron coincidence experiments of atoms and molecules

5D Microscopy

Chair: Christian Jung 14:00 - 16:10

FOREST SCIENCES 1005

5D1 Oliver Bunk (invited)

14:00 Multimodal imaging: bright-field, phase contrast and dark-field imaging of tissue samples

5D2 Alexander Gray

14:40 Depth resolved photoelectron microscopy of nanostructures via soft X-ray standing wave excitation

5D3 Toyohiko Kinoshita

14:55 Complete assignment of 3D spin axes of antiferromagnetic domains and domain walls of NiO by PEEM and cluster model calculation

5D4 Koji Horiba

15:10 Development of a three-dimensional scanning photoelectron microscope

5D5 Rainer Fink

15:30 Ultimate resolution soft X-ray microspectroscopy

5D6 Hyung Taek Kim

15:50 Single-shot nanometer-scale hologram using X-ray laser

POSTER SESSION 5P

Chair: Yongfeng Hu

EAST AND WEST ATRIA, LIFE SCIENCES CENTRE

16:10 - 18:00

Buses leave Walter Gage Residence between 18:45 - 19:15

CONFERENCE BANQUET

Vancouver Aquarium (Stanley Park)

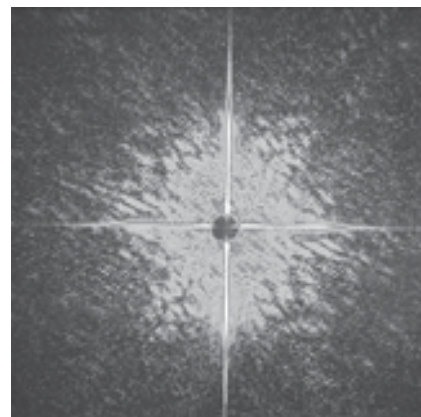
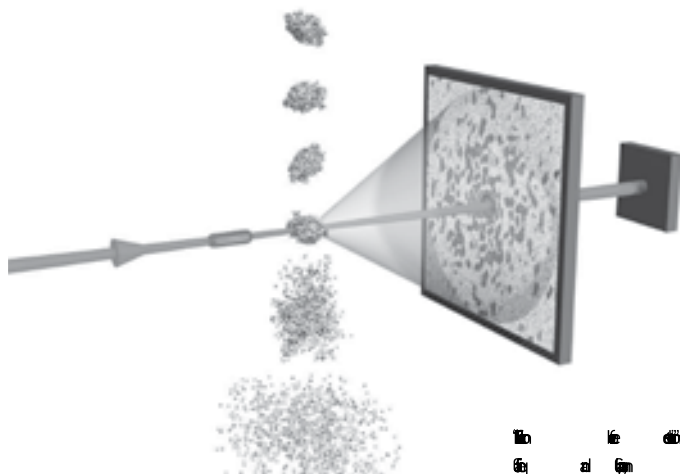
19:45 - 22:15

5PL1

Coherent X-ray Diffraction Imaging at the LCLS

Henry N. Chapman^{1,2}¹ Center for Free-Electron Laser Science, DESY, Hamburg, Germany.² University of Hamburg, Hamburg, Germany.

The ultrafast pulses from X-ray free-electron lasers are of high enough intensity and of sufficiently short duration that individual single-shot diffraction patterns can be obtained from a sample before significant damage occurs. This “diffraction before destruction” method may enable the determination of structures of proteins that cannot be grown into large enough crystals or are too radiation sensitive for high-resolution crystallography. In order to address the many challenges that we face in attempting molecular diffraction, we have carried out experiments in coherent diffraction from membrane protein nanocrystals at the Linac Coherent Light Source (LCLS) at SLAC. The periodicity of these objects gives us strong high-angle scattering signals in order to determine the effects of pulse duration and fluence on the high-resolution structure of single objects. The crystals are filtered to sizes less than 2 micron, and are delivered to the pulsed X-ray beam in a liquid jet. Snapshot diffraction patterns were recorded from individual crystals as small as 300 nm at the LCLS repetition rate with pnCCD detectors. It was possible to record millions of diffraction patterns, and we are assembling these data into 3D pattern for structure determination. This new form of protein nanocrystallography may open a new avenue for high-throughput membrane protein crystallography. Experimental data collection was carried out as part of a large collaboration, using the CAMP apparatus which was designed and built by the Max Planck Advanced Study Group at CFEL. The LCLS is operated by Stanford University on behalf of the U.S. Department of Energy, Office of Basic Energy Sciences.



“diffraction before destruction” by X-ray FEL pulses may overcome limitations of radiation damage. Chapman et al, Science 316, 1444 (2007); Chapman et al, Nat Phys 2, 839 (2006)



Henry Chapman received a PhD in Physics at the University of Melbourne in 1992, for the study of X-ray optics. This work earned him the Australian Institute of Physics Bragg Medal. While a postdoc at Stony Brook he performed the first demonstration of X-ray ptychography, developed X-ray imaging of labelled cells, and investigated coherent X-ray diffractive imaging with David Sayre. In 1995 he joined the nEUV lithography program at LLNL where he was instrumental in achieving the successful operation of an EUV prototype lithography system. He then returned to coherent X-ray imaging, carrying out experiments at the ALS in collaboration with Malcolm Howells (LBNL) and John Spence (ASU). In collaboration with a team from LLNL and Janos Hajdu of Uppsala University, he developed “diffraction before destruction” imaging at the FLASH FEL, at DESY in Hamburg. In 2007 he became one of the founding directors of the Center for Free-Electron Laser Science in Hamburg, where he is developing methods to image the structure and dynamics of proteins and other materials.

5PL2 (Invited)**Visualizing ultrafast chemical reactions by intense ultrashort laser pulses**A Hishikawa^{1,2}¹Department of Chemistry, Nagoya University, Nagoya, Japan; ²Institute for Molecular Science, Okazaki, Japan

Recent advances in laser technology have enabled us to utilize ultrashort intense laser pulses (<10 fs, $\sim 10^{15}$ W/cm²) as a new probe to visualize the ultrafast structural deformation in reaction processes. Molecules exposed to such intense laser pulses promptly eject several electrons by non-resonant interactions and undergo rapid bond breaking (called "Coulomb explosion") on the repulsive Coulombic potential energy surface of the highly charged states. Since the momenta of the resultant fragment ions reflect sensitively the geometrical structure of the target molecule, the Coulomb explosion provides direct access to the instantaneous structure in the course of reaction processes, as demonstrated for dissociating diatomic and triatomic molecules. Here we report real-time visualization of ultrafast hydrogen migration in acetylene dication by employing the pump-probe Coulomb explosion imaging. We also discuss the three-body Coulomb explosion of formaldehyde to understand the dynamics in intense laser fields and to seek the feasibility of applying the Coulomb explosion imaging to visualize the roaming hydrogen discovered recently in the UV photodissociation. A new approach using the high-order harmonics in the EUV ~ soft X-ray region to probe the ultrafast molecular dynamics with an unprecedented time resolution is also presented. Preliminary pump-probe experiments on the photodissociation of Br₂, Br₂ + 400nm \rightarrow Br₂(C¹ π_u) \rightarrow Br(2P_{3/2}) + Br(2P_{3/2}), show a steep rise (~ 80 fs) of the Br(2P_{3/2}) yields, reflecting a ultrashort pulse duration (<20 fs) of the 27th harmonic pulses used to probe the Br(2P_{3/2}) product. Full characterization of the temporal profile of the harmonic pulse and application to the time-resolved photoelectron imaging are in progress.

LIFE SCIENCES INSTITUTE 2

10:40-12:30

5A1 (Invited)**Status of the SCSS X-ray Free Electron Laser XFEL/SPring-8 Project in Japan**T Shintake¹¹RIKEN, SPring-8, Sayo, Hyogo, Japan

The XFEL/SPring-8 is under construction, aiming at generating 10 GW peak 1 Angstrom coherent radiation in early 2011. Using 8 GeV C-band high gradient accelerator and short period undulator, the total system fits within available site length of 700 m at SPring-8. Tunnel construction was completed in March 2009 and after one year most of all accelerator columns have been installed. Machine commissioning is scheduled from September 2010, and we expect first light from the undulator in March 2011. The machine will provide intense coherent X-ray in short bunch train up to 50 bunches in 60 pulse/sec (3000 bunch/sec). Minimum bunch length is 10 femtosec, which allow research on the ultra-fast science.

5A2

The European XFEL project: status and research applications

S Molodtsov¹

¹European XFEL GmbH, Hamburg, Germany

The European XFEL is a new international research installation that is currently under construction in the Hamburg area in Germany. The facility will generate new knowledge in almost all the technical and scientific disciplines that are shaping our daily life – including nanotechnology, medicine, pharmaceuticals, chemistry, materials science, power engineering and electronics. The X-ray flashes will be produced in a 3.4-kilometre-long facility. Most of it will be housed in tunnels deep below ground. Three sites will provide access to the tunnels and the experiment stations. In its start-up configuration, the European XFEL will comprise 3 different light sources – undulators operating at a fixed energy 12.4 keV (SASE 1), as well as in energy ranges 3.1 – 12.4 keV (SASE 2) and 0.2 – 3.1 keV (SASE 3), respectively. Six experimental stations optimized for particular purposes will be installed. Each experiment requires light with special properties, such that the stations are permanently assigned to the different light sources (beamlines) of the European XFEL. On 8 January 2009, civil engineering work (tunnels, shafts, halls) has been started at all three construction sites. In this presentation status and further parameters of the European XFEL facility as well as planned research applications are reviewed.

5A3

keV high harmonic and K-shell excitation using 2-cycles IR (2.1 μ m) radiation source

G Marcus,¹ W Helml,¹ X Gu,¹ Y Deng,¹ R Hartmann,² R Kienberger,^{1,3} F Krausz^{1,4}

¹Max-Planck-Institute of Quantum Optics, Garching, Germany; ²Halbleiterlabor, Max Planck Institute, München, Germany;

³Department of Physics, Technische Universität München, Garching, Germany; ⁴Department of Physics, Ludwig-Maximilians-Universität München, Garching, Germany

Most of the processes during the interaction of ultra-fast laser with matter are intuitively described with the three step model. In this model, the strong electric field of the laser distorts the atomic field in such a way that an electron can tunnel out of the atom and emerge at the continuum with zero velocity. Next to that, the electron accelerates in the laser's electric field, driven back with an excess energy and re-collides with its parent atom. The outcome of this laser induced re-collision (LIR) may branch into few possible channels: **a)** inelastic scattering of the electron which leads to a typical discrete spectrum of electrons known as above-threshold-ionization (ATI), **b)** excitation/ionization of the ion, **c)** recombination of the electron with the parent ion and the release of the excess energy in a form of XUV radiation in a process known as high-harmonic-generation (HHG). All of the above mentioned processes are key tools in the fast developing femto and attosecond science. Here we describe the use of a unique 2-cycle IR ($\lambda_0=2.1\mu\text{m}$) radiation source built by us to generate high harmonics up to 1.7keV and the observed K-shell excitation by the re-colliding electron in atoms and molecules. The results and future perspective will be discussed.

5A4

News and views from the attosecond generation, characterization and applications frontier

P Tzallas,¹ J Kruse,^{1,2} E Skatzakis,^{1,2} Y Nomura,³ R Hoerlein,³ C Kalpouzos,¹ G Tsakiris,³ D Charalambidis^{1,2}

¹FORTH-IESL, Heraklion, Greece; ²Department of Physics, Univ. of Crete, Heraklion, Greece; ³Max-Planck-Institut für Quantenoptik, Garching, Germany

We report on recent results in the generation, characterization and applications of attosecond pulse trains and ultra-broad coherent XUV continua: 1) Generation: 1a) We report experimental results confirming contribution of both long and short trajectories in on-axis harmonic generation before, at and after an atomic gas jet, i.e. under three different phase matching conditions. The contribution of both trajectories is manifested through their interference leading to a modulated harmonic (and side band) yield as a function of the driving intensity. 1b) We report the generation of sub-fs pulse trains from laser surface plasma measured through 2nd order intensity volume autocorrelation (2nd order IVAC). 2) Characterization: We present comparative studies between RABITT and 2nd order IVAC in on axis harmonic generation before, at and after an atomic gas jet. We find that the two techniques give fairly different results that are compatible with the differently weighted but unavoidable presence of the long and short trajectory in the generation process in all three phase matching conditions. We show that the relative contributions of the two trajectories can be estimated through RABITT measurements, while spatiotemporal mean pulse durations can be extracted from 2nd order IVAC traces. 3) Applications: 3a) We present time resolved spectroscopy at the 1fs temporal scale and ultra-broad band XUV Fourier Transform Spectroscopy in a manifold of doubly excited autoionizing and inner-shell Auger decaying states excited simultaneously through a coherent broadband XUV continuum.

5A5

Time-resolved photoelectron diffraction on laser-aligned molecules

D Rolles,^{1,2} A Rudenko,^{1,3} S Epp,^{1,3} L Foucar,^{1,2} B Rudek,^{1,3} B Erk,^{1,3} F Krasniqi,^{1,2} R Hartmann,^{1,4} N Kimmel,⁴ G Weidenspointer,⁴ L Strüder,^{1,4} S Schorb,⁵ M Adolph,⁵ T Gorkhover,⁵ J Thogersen,⁶ L Holmegaard,⁶ J Maurer,⁶ P Johnsson,⁷ A Rouzee,⁸ C Bostedt,⁹ R Coffee,⁹ J Bozek,⁹ J Schulz,¹⁰ L Gumprecht,¹⁰ A Aquila,¹⁰ S Stern,¹⁰ N Coppola,¹⁰ H Chapman,¹⁰ J Küpper,¹¹ F Filsinger,¹¹ KU Kühnel,³ R Moshhammer,^{1,3} I Schlichting,^{1,2} J Ullrich^{1,3}

¹Max Planck Advanced Study Group at CFEL, Hamburg, Germany; ²Max-Planck-Institut für medizinische Forschung, Heidelberg, Germany; ³Max-Planck-Institut für Kernphysik, Heidelberg, Germany; ⁴Max Planck Halbleiterlabor, München, Germany; ⁵Technische Universität Berlin, Berlin, Germany; ⁶Department of Chemistry, Aarhus University, Aarhus C, Denmark; ⁷Atomic Physics, Lund University, Lund, Sweden; ⁸FOM AMOLF, Amsterdam, Netherlands; ⁹LCLS, Menlo Park, CA, United States; ¹⁰CFEL, Deutsches Elektronen Synchrotron, Hamburg, Germany; ¹¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The photoelectron angular distributions of laser-aligned di-iodobenzene and carbonyl sulfide molecules were measured at the Linac Coherent Light Source (LCLS) using a velocity map imaging spectrometer. The molecules were adiabatically aligned by a nano-second YAG laser synchronized with the FEL and, in addition, could also be dissociated by a fs-Ti:Sa laser pulse prior to the FEL ionization, thus allowing time-resolved photoelectron diffraction measurements of dissociating molecules.

FOREST SCIENCES CENTRE 1005

10:40-12:30

5B1 (Invited)**Magnetic soft X-ray microscopy – achievements and future opportunities to image fast spin dynamics in nanomagnetism**P Fischer¹¹CXRO, LBNL, Berkeley, CA, United States

The scientific desire and technological demand to manipulate spins on the nanoscale e.g. in spintronic applications can only be met by advanced analytical tools. The ultimate goal for modern magnetic microscopies is to combine spatial resolution in the nanometer regime, a time resolution on a ps to fs scale and elemental specificity which allows to study novel multicomponent and multifunctional magnetic nanostructures and their ultrafast spin dynamics down to fundamental magnetic length and time scales. Magnetic soft X-ray microscopy using Fresnel zone plate as X-ray optical elements provides a spatial resolution down to nearly 10nm with a temporal resolution below 100ps, which is limited by the inherent time structure of current X-ray sources available at synchrotrons. X-ray magnetic circular dichroism serves as element specific and strong magnetic contrast mechanism. Current research with X-ray microscopy focuses on spin torque and external field driven nanoscale magnetic dynamics of vortex cores and domain walls, field driven domain wall propagation in nanowires and the stochastic behavior of magnetization reversal throughout the hysteresis cycle, such as nucleation and Barkhausen avalanche processes. Next generation X-ray sources will provide sufficient photons per X-ray pulse to enable snapshot imaging of fsec spin dynamics at the nanoscale.

This work is supported by the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231.

5B2**Depth-resolved magnetism and valence band densities of states for the magnetic tunnel junction interface Fe/MgO via standing-wave excited photoelectron emission and magnetic circular dichroism**C Papp,^{1,2,3} B Balke,^{1,2,4} SH Yang,⁵ S Döring,⁶ U Berges,⁶ F Schonbohm,⁶ AX Gray,^{1,2} BC Sell,⁷ M Gorgoi,⁸ D Buegler,⁹ JB Kortright,² CM Schneider,⁹ C Westphal,⁶ CS Fadley^{1,2}

¹Department of Physics, University of California, Davis, CA, United States; ²Material Sciences Division, LBNL, Berkeley, CA, United States; ³Physical Chemistry II, University of Erlangen, Erlangen, Germany; ⁴Institut für Anorganische und Analytische Chemie, J. Gutenberg-Universität, Mainz, Germany; ⁵IBM Almaden Research Center, San Jose, CA, United States; ⁶Exp. Physik 1 and DELTA, TU Dortmund, Dortmund, Germany; ⁷Physics Dept., Otterbein College, Westerville, OH, United States; ⁸BESSY, Helmholtz Center Berlin, Berlin, Germany; ⁹Jülich Research Center, Jülich, Germany

The depth-resolved chemical, magnetic, and electronic structure properties of an Fe/MgO magnetic tunneling junction were investigated using standing-wave excited photoelectron emission with magnetic circular dichroism. Standing-wave-induced modulations of core and valence-band intensities were measured, including MCD measurements of the Fe 2p level. The experimental results were compared to X-ray optical theoretical calculations in order to quantitatively derive the depth dependence of concentration and Fe magnetization. Furthermore, depth-resolved valence-band densities of states have been determined via a self-consistent deconvolution of the soft X-ray wedge-scan data; these results suggest oxidation of Fe at the interface.

This work was supported by the Humboldt foundation, the Helmholtz Association, and the U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

5B3

Responses of an ultrathin cobalt film in contact with an organic pentacene layer

DH Wei,¹ YL Chan,¹ YJ Hung,^{1,2} CH Wang,^{1,2} YC Lin,¹ CY Chiu,¹ YL Lai,¹ HT Chang,^{1,2} CH Lee,^{1,2} YJ Hsu^{1,3}

¹Scientific Research Division, National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan; ³Institute of Electro-Optical Science and Engineering, National Cheng Kung University, Tainan, Taiwan

One obstacle hindering the development of organic spintronics is the loss of magnetoresistance (MR) at a temperature much lower than the Curie temperature of ferromagnetic (FM) electrodes in used. [1] As the population of spin-polarized carriers is clearly not in the shortage, it was suggested that the spin transport efficiency could be somehow altered at the interfaces of FM-organic hybrid structure [2]. To gain the much needed insights, we fabricate two series of ultrathin pentacene/cobalt (Pn/Co) and cobalt/pentacene (Co/Pn) bilayers under ultra-high vacuum condition to emulate the interfacial regions of a Co/Pn/Co spin-valve structure. Employing the magneto-optical Kerr effect (MOKE) measurements, photoemission spectroscopy and microscopy, we found, in a Co/Pn/Co trilayers, the layer symmetry does not necessarily warrant a magnetic symmetry between its two interfaces. In this presentation, we discuss the origins, as well as the implications, of having such interfacial disparities occurred in a vertical spin-valve structure. [3]

[1] Z. H. Xiong, *et al.*, *Nature* **427**, 821 (2004).

[2] V. A. Dediu, *et al.*, *Nature Mater.* **8**, 707 (2009).

[3] Yuet-Loy Chan, *et al.*, *Phys. Rev. Lett.* (2010).

5B4

Slow dynamics in Au/Co/Au thin films near the spin-reorientation transition

S Roy,¹ KA Seu,^{1,2} D Parks,² R Su,² JJ Turner,³ S Park,⁴ CM Falco,⁵ S Kevan²

¹Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States; ²Dept. of Physics, University of Oregon, Eugene, OR, United States; ³LCLS, SLAC National Accelerator Laboratory, Menlo Park, CA, United States; ⁴Pusan National University, Busan, Republic of Korea; ⁵Optical Sciences Center, University of Arizona, Tucson, AZ, United States

Ultrathin magnetic films sometimes exhibit a spin reorientation transition (SRT) where the magnetization changes its preferred direction from in-plane to out-of-plane or *vice-versa*. The SRT can happen as a function of the thickness of the magnetic film or as a function of temperature. Around the SRT temperature the in-plane structure could be complex due to coexisting phases or canted magnetization phases. It is predicted that fluctuation could play an important role in such phases. Using coherent resonant soft X-ray scattering, we have performed photon correlation spectroscopy measurements of slow magnetization fluctuations in an ultrathin Au/Co/Au system that exhibits an SRT as a function of temperature. The intermediate scattering function is well described by a stretched exponential that is indicative of cooperative motion throughout the temperature range of 150 - 300 K. The decay times were found to exhibit a maximum at the transition temperature. We also determine the anisotropy space phase diagram which allows us to predict the phases of the system during the spin reorientation transition. Our results show that slow dynamics in the mesoscopic length scale can provide valuable insights into the nature of magnetic phase transitions. Work at LBNL is supported by DOE.

5B5

MCD study on Ce@C₈₂ and Ce₂@C₈₀ in the soft X-ray regionJ Ishikawa,¹ T Miyahara,² Y Hirato,¹ H Ishii,¹ T Kodama,³ K Kikuchi,³ T Nakamura,⁴ K Kodama,⁴ D Asakura,⁵ T Koide⁵¹Department of Physics, Tokyo Metropolitan University, Hachioji-shi, Tokyo, Japan; ²Department of Mathematical and Physical Sciences, Japan Women's University, Bunkyo-ku, Tokyo, Japan; ³Department of Chemistry, Tokyo Metropolitan University, Hachioji-shi, Tokyo, Japan; ⁴Spring-8, Sayo-gun, Hyogo-ken, Japan; ⁵Photon Factory, Tsukuba-shi, Ibaraki-ken, Japan

We have measured the temperature dependence of magnetic circular dichroism of Ce atoms encapsulated in C₈₂ and C₈₀ in the Ce 3d-4f excitation region. From the gradient of the Curie-Weiss plot of the data are estimated the magnetic moments in the low temperature (< 20 K) and high temperature (>20 K) regions. A fullerene C₈₀ includes two Ce atoms in the cage and they are supposed to move in the cage avoiding each other, while C₈₂ contains just one Ce atom in the cage. The moment of Ce 4f states in C₈₀ was found to be 0.75 μ_B in the low temperature and 0.51 μ_B in the high temperature region, which are much smaller than the Hund-coupled ground state moment, but the Weiss temperature was found to be positive, suggesting ferromagnetic coupling between two Ce atoms. The reduction of the moment at high temperature suggests more rapid motion of Ce atoms in the cage. The moment of a Ce 4f electron in C₈₂ was estimated to be 0.82 μ_B below 20 K and 0.99 μ_B above 20 K but it showed a slightly negative Weiss temperature, suggesting antiferromagnetic behaviour extending two cages, probably through weak RKKY interaction. However through the spectral profile showed that the hybridization between Ce 4f and C π states is negligibly small. The small magnetic moment may be attributed to reduction of 4f orbital momentum caused by an effective crystal field, which is different between C₈₂ and C₈₀. We have also measured XAS spectra on Ce@C₈₂ in the C 1s excitation region. The similar XAS measurements were performed on C₆₀, C₇₀, and Dy@C₈₂ encapsulated in a single-wall carbon nanotube, exhibiting an interesting behaviour of fullerene-nanotube interaction.

LIFE SCIENCES INSTITUTE 2

14:00-16:10

5C1 (Invited)

Molecular inner-shell spectra of weakly bonding and interacting systemsN Kosugi¹¹Institute for Molecular Science, Myodaiji, Okazaki, Japan

Recently 1 meV energy resolution is achievable even in soft X-ray spectroscopy. This means that we can observe and discuss weak molecular interaction in *weakly bonding and interacting systems*. Cluster-induced energy shift, in addition to newly allowed states such as surface-induced and inter-site Auger transitions, is interesting in inner-shell ionization and excitation. There are several kinds of origins to give the energy shift. In the case of X-ray photoelectron spectroscopy (XPS), an ionized molecule is stabilized by induced polarization (PL) screening of surrounding molecules. This phenomenon explains redshift in the inner-shell ionization energy of clusters in comparison with a free system. However, polar surrounding molecules are not always aligned to stabilize the ionized molecule. That is, the redshift of the inner-shell ionization energy is not always obvious in polar systems. On the other hand, in the case of X-ray absorption spectroscopy (XAS), the excited electron is bound by an excited molecule in clusters, and directly interacts with the surrounding molecules. This interaction corresponds to the exchange (EX) repulsion arising from the Pauli exclusion principle.

We would like to acknowledge great contributions of collaborators to the present work, especially, Mananari Nagasaka, Takaki Hatsui, and Eckart Rühl.

5C2

Dynamics of terminal atom migration and dissociation in small core-excited molecules probed by multiple ion momentum imaging

J Laksman,¹ D Céolin,¹ M Gisselbrecht,¹ SL Sorensen¹

¹Synchrotron Radiation Research, Lund, Sweden

With our in-house built momentum imaging spectrometer, we have performed studies that focus on rapid geometry change near the carbon 1s edge in the three different linear molecules: ethyne, carbon dioxide and carbonyl sulfide that all have carbon as center atoms. The core-excited state decays rapidly via Auger transitions, which populate electronic states in the dication, and dissociation to two or more fragments can result. By analyzing the momenta of all fragments produced in dissociation we can filter out events connected with isomerization and deformation from the linear geometry. We discuss two-body dissociation of the dications in the context of fast migration of terminal atoms, focusing on the H_2^+/C_2^+ , O_2^+/C^+ and OS^+/C^+ fragmentation channels, that are fingerprints of deformation. We find that these channels have strong resonance dependence and appear mainly at the C 1s $\rightarrow \pi^*$ resonance. Our spectrometer provides us with complete angular information that allows us to estimate the fragments β -parameter. We present evidence for a strong anisotropy in the production of these fragments through a rapid deformation of the molecule to a dibridged conformation with the transition dipole moment parallel to the polarization of the exciting radiation.

5C3

Photodissociation dynamics of the chloroform molecule excited in the vicinity of the Cl 1s edge

AF Lago,¹ GGB de Souza,² ACF Santos,³ AS Schlachter,⁴ RL Cavasso-Filho¹

¹Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André- SP, Brazil; ²Instituto de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro- RJ, Brazil; ³Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro- RJ, Brazil; ⁴Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley-CA, USA

The photo-fragmentation of the chloroform ($CHCl_3$) molecule has been investigated near the Cl K edge using ion yield spectroscopy, electron-ion coincidence and synchrotron radiation. Total and partial ion yield and mass spectra have been recorded as function of the photon energy. Several singly and multiply charged ions have been identified, including the following anions (Cl^- , H^- , C^-). This work provides the first experimental report of negative ion formation from the dissociative photoionization of the chloroform molecule following excitation in the vicinity of the Cl K shell. Striking differences in the ion yield spectra for the anions have been observed and discussed in a comparative way. The spectra were dominated by atomic singly and multiply-charged fragments. The fragmentation processes were governed by complex decay mechanisms involving singly and multiply charged species formed below and above the ionization threshold, as well as via dissociation into ion pairs. Our new PEPICO and PEPIPCO results supplement the analysis and assignment obtained from the ion yield spectra and also present evidences of preservation of molecular alignment for the $CHCl_3$ molecule upon resonant core-electron excitation at the Cl K shell. This work was financially supported by FAPESP, FAPERJ and CNPq (Brazil), and the U.S. Department of Energy.

5C4

Sequential multi-photon multiple-ionization of molecules by EUV free-electron laser at SPring-8

A Yamada,^{1,2} H Fukuzawa,^{1,2} K Motomura,^{1,2} XJ Liu,^{1,2} C Wang,^{1,2} L Foucar,^{1,2,3} M Kurka,^{1,2,4} M Okunishi,¹ K Ueda,^{1,2} N Saito,^{2,5} H Iwayama,^{2,6} K Nagaya,^{2,6} H Murakami,^{2,6} A Sugishima,^{2,6} M Yao,^{2,6} A Rudenko,^{2,3,4} KU Kühnel,^{2,3} J Ullrich,^{2,3,4} R Feifel,^{2,7} A Czasch,⁸ R Dörner,⁸ M Nagasono,² A Higashiya,² T Togashi,^{2,9} K Tono,² M Yabashi,² T Ishikawa,² H Ohashi,^{2,9} H Kimura^{2,9}

¹IMRAM, Tohoku University, Sendai, Japan; ²RIKEN, XFEL Project Head Office, Sayo, Japan; ³Max-Planck Advanced Study Group at CFEL, Hamburg, Germany; ⁴Max-Planck-Institut für Kernphysik, Heidelberg, Germany; ⁵National Metrology Institute of Japan, AIST, Tsukuba, Japan; ⁶Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan; ⁷Department of Physics and Material Science, Uppsala University, Uppsala, Sweden; ⁸Institut für Kernphysik, Universität Frankfurt, Frankfurt, Germany; ⁹Japan Synchrotron Radiation Research Institute, Sayo, Japan

Free-electron lasers (FELs) based on self-amplified spontaneous-emission (SASE) in the extreme ultraviolet (EUV) region have proven to be a powerful tool to explore the interaction of strong EUV laser pulses with atoms, molecules and clusters. We have investigated multiple ionizations of N₂, O₂ and CO₂ molecules irradiated by 20 eV and 24 eV EUV-FEL pulses from SPring-8 Compact SASE Source (SCSS) test accelerator by means of three dimensional coincidence ion momentum spectroscopy. We measured kinetic energy release (KER) distributions of multiply charged (up to 5+ or 6+) molecular ions. The KER distributions indicate that the internuclear distance is elongated during the multiple ionization processes, suggesting that the ionizations to the highly charged N₂, O₂ and CO₂ molecules are “sequential” multi-photon absorption processes. We are grateful to the SCSS test accelerator operation group at RIKEN for continuous support in the course of the studies.

5C5

Electronic properties of thin magnetic films probed by Auger photoelectron coincidence spectroscopy (APECS)

G Stefani,¹ R Gotter,² F Offi,¹ F Da Pieve,¹ S Ugenti,¹ RA Bartynski,³ G Fratesi,⁴ M I Trioni⁵

¹Dipartimento di Fisica and CNISM, Università Roma Tre, Roma, Italy; ²IOM-CNR, Basovizza, Trieste, Italy; ³Department of Physics and Astronomy and Laboratory of Surface Modification, Rutgers University, Piscataway, United States; ⁴Dipartimento Scienza dei Materiali, Università Milano Bicocca, Milano, Italy; ⁵CNISM and CNR, UdR Milano Bicocca, Milano, Italy

The dichroic effect recently discovered in Auger-photoelectron coincidence spectroscopy (DEAR-APECS) has been suggested as a suitable tool to study complex systems such as magnetic thin films and multilayers. We present clear experimental evidences for such a dichroic effect in M₃VV Auger line shape of Co and Fe films on Cu(001) as measured by angle resolved APECS. The high degree of flexibility in experimental configurations available at the ALOISA beam-line (ELETTRA, Trieste) provides access to the final state spin selectivity (triplet vs. singlet components) highlighted by the present results. Due to the very high statistics achieved in the measurement, some finer details can be resolved at energies corresponding to transitions involving electrons from the top and the bottom of the valence band, when comparing singlet versus triplet contributions. As a first attempt and in the simplest approach, the observed dichroism can be explained by a theoretical simulation performed in the Density Functional Theory framework. Using the Fermi Golden rule, the Auger spectrum and its angular distribution can be computed. For magnetic systems, the spin dependence of the Auger matrix elements allows to work out the triplet/singlet contributions to the Auger spectrum whose angular distribution follows a non-trivial behaviour, in case of non-spherical ionized core level (e.g. l=1, m=0).

5C6

Multi-electron coincidence experiments of atoms and molecules**R Feifel¹**¹Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

To obtain triple ionization spectra and reliable triple ionization energies of atoms and molecules we detect and measure in coincidence all three electrons emitted in photoionization. This can most easily be done by making use of the double Auger effect at photon energies above inner shells where triple ionization is relatively abundant. The magnetic bottle apparatus gathers more than 90 % of photoelectrons from a point source and directs them to a 2.2 m distant detector where their flight times are recorded. The numerical resolution $E/\Delta E$ is about 50 and detection efficiency is independent of electron energy up to about 200 eV. In this talk, I will present a selected choice of examples in order to demonstrate the capability of this technique. In particular for the molecular cases, we obtained the first ever triple ionization electron spectra. The molecules studied so far include N_2 , CO, NO, O_2 , N_2O , CH_4 , CO_2 , CS_2 , OCS, H_2S , etc. The OCS^{3+} and CS_2^{3+} are particularly interesting as being stable on the mass spectrometer time scale. Our spectra show that this stability is a property of the molecular ion ground states with the outer valence configuration $\epsilon s^2 p^4$. We have calculated the energies of the higher states of OCS^{3+} using high-level quantum chemical methods. Comparison with the measured spectrum shows that in triple photoionization of closed shells, doublet states of the final ion are preferred over quartets, and the strongest transitions arise from simple removal of three electrons from the occupied orbitals.

FOREST SCIENCES 1005

14:00-16:10

5D1 (Invited)

Multimodal imaging: bright-field, phase contrast and dark-field imaging of tissue samples**O Bunk¹**¹Paul Scherrer Institut, Villigen PSI, Switzerland

The complementarity and overlap of four X-ray imaging techniques is described and illustrated with tissue samples like brain, teeth and bone. The techniques are: 1. Scanning X-ray transmission microscopy (STXM) with a pixelated detector for obtaining both absorption and differential phase contrast. 2. Scanning X-ray diffraction microscopy (SXDM, CDI) for high-resolution imaging. 3. Small-angle X-ray scattering (scanning SAXS) in scanning mode for recovering the density, degree of orientation anisotropy, and orientation of structures in the nanometer range spatially resolved over extended samples of several square millimeters or even centimeters. 4. Absorption, differential phase contrast and dark field imaging with a grating interferometer for X-ray computed tomography (CT) measurements. The focus will be on scanning SAXS as a bridge between high-resolution small field-of-view techniques like electron microscopy and SXDM, and low-resolution large field-of-view techniques, like micro X-ray CT. All techniques can be applied for retrieving three-dimensional information in a computed tomography approach. Recent applications will be shown. While the biomedical examples in this presentation touch on fields like cancer, osteoporosis, and carious research, the techniques are well suited for materials science applications as well.

5D2

Depth resolved photoelectron microscopy of nanostructures via soft X-ray standing wave excitation

F Kronast,¹ AX Gray,^{2,3} C Papp,^{2,3,4} S H Yang,⁵ A Kaiser,⁶ S Cramm,⁶ IP Krug,⁶ F Salmassi,⁷ E M Gullikson,⁷ DL Hilken,⁷ EH Anderson,⁷ P Fischer,³ HA Dürr,¹ CM Schneider,⁶ CS Fadley^{2,3}

¹Helmholtz-Zentrum Berlin - BESSY II, Berlin, Germany; ²Department of Physics, University of California, Davis, CA, United States;

³Materials Sciences Division, LBNL, Berkeley, CA, United States; ⁴Physical Chemistry II, University of Erlangen, Erlangen, Germany;

⁵IBM Almaden Research Center, San Jose, CA, United States; ⁶Jülich Research Center, Jülich, Germany; ⁷Center for X-ray Optics, LBNL, Berkeley, CA, United States

We demonstrate the addition of depth resolution to the usual two-dimensional images in photoelectron emission microscopy (PEEM), with application to a square array of circular magnetic Co microdots. The method is based on excitation with a soft X-ray standing-wave (SW) generated by Bragg reflection from a multilayer mirror substrate. The standing wave is moved vertically through the sample simply by varying the photon energy around the Bragg condition. The experiment was conducted at the soft X-ray beamline UE49-PGM-a of the storage ring BESSY-II (Helmholtz Zentrum Berlin) that is equipped with an Elmitec PEEM-II including an integrated photoelectron energy analyzer. Depth-resolved PEEM images were obtained for all of the observed elements. Photoemission intensities as functions of photon energy were compared to X-ray optical theoretical calculations in order to quantitatively derive the depth-resolved film structure of the sample. This SW approach thus provides complementary information to the usual lateral information provided by the PEEM, and should have wide applicability to studies of magnetic nanostructures in the future.

Funded by the Humboldt foundation and the U.S. Department of Energy [DE-AC02-05CH11231].

5D3

Complete assignment of 3D spin axes of antiferromagnetic domains and domain walls of NiO by PEEM and cluster model calculation

K Arai,¹ T Okuda,² A Tanaka,³ M Kotsugi,^{4,6} K Fukumoto,⁴ T Ohkouchi,⁴ T Nakamura,⁴ T Muro,⁴ T Matsushita,⁴ M Oura,⁵ Y Senba,⁴ H Ohashi,⁴ A Kakizaki,¹ T Kinoshita^{4,6}

¹Inst. Solid State Phys., Univ. Tokyo, Kashiwa, Japan; ²HiSOR, Hiroshima Univ., Higashihiroshima, Japan; ³ADSM, Hiroshima Univ., Higashihiroshima, Japan; ⁴JASRI/SPring-8, Sayo, Japan; ⁵RIKEN/SPring-8, Sayo, Japan; ⁶CREST-JST, Kawaguchi, Japan

NiO is known as one of the typical antiferromagnetic (AF) materials. Existence of very complicated domain structures is suggested, namely, 4 twin-domains (T-domain), 12 spin-domains (S-domain) and several types of domain-walls. It is well known that the combination method of photoemission electron microscope (PEEM) and X-ray magnetic linear dichroism (MLD) gives us detailed information of the AF domain structures [1]. Although many studies have been done, the perfect assignment of the spin orientation of all the domain structures has not been reported. We have successfully assigned the three-dimensional (3D) spin axes of whole AF domain structures of NiO single crystal by PEEM study using MLD at Ni L_2 edge and nonmagnetic linear dichroism (LD) at O K edge [2]. From the comparison of the PEEM contrast as a function of the angle between the polarization vector and the crystal axes with the cluster model calculation (analytic solution) including the crystal symmetry, the 3D spin orientations in all the domains and the domain-walls could be completely determined. This analytic solution is very essential for understanding the behavior of MLD in NiO. We further observed the width of all the T- and S-walls. The results would give us an important basis for understanding of antiferromagnetism, exchange bias in spin valve system, and so on.

[1] For example, H. Ohldag *et al.*, Phys. Rev. B **79**, 052430 (2009), and references therein.

[2] K. Arai *et al.*, J. Phys. Soc. Jpn. **79**, 013703 (2010).

5D4

Development of a three-dimensional scanning photoelectron microscope**K Horiba,^{1,2,3} Y Nakamura,¹ S Toyoda,^{1,2,3} H Kumigashira,^{1,2,4} M Oshima,^{1,2,3} K Amemiya^{3,5}**

¹Department of Applied Chemistry, The University of Tokyo, Tokyo, Japan; ²Synchrotron Radiation Research Organization, The University of Tokyo, Tokyo, Japan; ³CREST, Japan Science and Technology Agency (JST), Tokyo, Japan; ⁴PRESTO, Japan Science and Technology Agency (JST), Saitama, Japan; ⁵Photon Factory, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Japan

In order to achieve nondestructive observation of three-dimensional spatially resolved electronic structure in solids, we develop a new scanning photoelectron microscope system combined with depth profiling in electron spectroscopy for chemical analysis (ESCA). We call this system "3D nano-ESCA". For the X-ray focusing optics, a Fresnel zone plate (FZP) is used. The diameter and the outermost zone width of FZP are 200 microns and 35 nanometers, respectively. In order to obtain angular dependence of photoelectron spectra without any sample rotating motion for depth profiling analysis using the maximum entropy method, we select a VG-Scienta R3000 analyzer with the wide-angle lens as a high-resolution angle-resolved electron spectrometer. The system has been installed at a new University-of-Tokyo Materials Science Outstation beamline BL07LSU of SPring-8 and the total spatial resolution of 92 nm is achieved.

5D5

Ultimate resolution soft X-ray microspectroscopy**R Fink,¹ J Raabe,² I Schmid,² C Hub,¹ S Wenzel¹**

¹Univ. Erlangen-Nuremberg, Physical Chemistry and ICMM, Erlangen, Germany; ²Paul-Scherrer-Institut, SLS, Villigen, Switzerland

Zone-plate based microspectroscopes are currently installed at all major synchrotron facilities. Based on recent improvements in the fabrication of nanoscaled zone-plates with high aspect ratios lateral resolutions on the order of about 10 nm were achieved. We have set up two spectromicroscopes at bending magnet beamlines of the Swiss Light Source (SLS), which offer versatile experimental opportunities for thin film analysis at ultimate resolution. The PolLux-STXM is a state-of-the-art scanning transmission X-ray microspectroscopy. It includes different contrast modes like phase contrast or surface-sensitive detection modes using the parallel detection of secondary electrons emitted from the irradiated spot. NanoXAS is a combined STXM and AFM, thus offering direct correlation of chemical and morphological properties. A modified conductive AFM-tip even allows spatial resolutions below the diffraction limit of the STXM zone plate (goal: 6 nm). We report on recent applications of these instruments with particular emphasis on in-situ variations, e.g., operation of organic field-effect transistors or solar cells or thermo-responsive microgels. Chemical or electronic modifications are monitored by the spectral changes in the NEXAFS fine structures. Some other prototype experiments include proton-irradiated graphene-layers, polymer blends and block copolymer films, environmentally relevant materials, nanoparticles, or magnetic nanostructures. In the latter case, time-resolved studies with picosecond resolutions are combined with highest spatial resolution to study magnetization dynamics in confined magnetic structures.

The project is funded by the BMBF [project 05 KS7WE1].

5D6

Single-shot nanometer-scale hologram using X-ray laser**HT Kim,¹ IJ Kim,¹ CM Kim,¹ TJ Yu,¹ SK Lee,¹ JH Sung,¹ JW Yoon,¹ H Yun,¹ TM Jeong,¹ IW Choi,¹ J Lee¹**¹Center for Femto-Atto Science and Technology, and Advanced Photonics Research Institute, GIST, Gwangju, Republic of Korea;²Department of Physics, KAIST, Daejeon, Republic of Korea

Nano-imaging techniques with single exposure have become importance issues due to its potential to reveal structural the dynamics of nano-materials. X-ray free electron laser has a great potential in the single-shot nano-imaging due to its enormous output power and short pulse duration [1]. However, the free electron lasers are very huge facility compared to the X-ray sources driven by table-top high power lasers. Recently, table-top X-ray sources, such as X-ray lasers and high-order harmonics, using ultrashort intense lasers have been achieved high photon flux and quality enough for nano-imaging techniques. In this presentation, we will report on single shot X-ray hologram with nanometer scale resolution using Ni-like Ag X-ray laser driven by a 10-Hz Ti:Sapphire laser system at the Advanced Photonics Research Institute (APRI). Recently, we have succeeded in saturating Ni-like Ag X-ray laser at 13.9-nm wavelength using a variant of GRIP geometry pumped by single-profiled pump laser pulse [2]. Using the Ni-like Ag X-ray laser, we succeeded in obtaining lensless Fourier holograms [3,4] with a single exposure of X-ray laser pulse. The reconstructed image has a resolution of around 100 nm. This technique can realize the time-resolved nano imaging with picosecond temporal resolution and nanometer spatial resolution that can provide a new inspection method in material science and bio science.

[1] H. N. Chapman et al., *Nature Physics* 2, 839 (2006).

[2] H. T. Kim et al., *Phys. Rev. A* 77, 023807 (2008).

[3] G. W. Stroke, *Appl. Phys. Lett.* 6, 210 (1965).

[4] S. Eisebitt et al., *Nature* 432, 885 (2004).

Poster Session 5P

5P - Thursday, July 15, 16:10-18:00

[Setup by 10:40 on Wednesday, July 14, take down by 16:00 on Friday, July 16]

The Poster Sessions take place in the East and West Atria of the Life Sciences Institute. The conference will not be responsible for posters that are left up after the above take down times.

5P Session Topic Breakdown

ATOMIC, MOLECULAR, OPTICS – EXPERIMENTAL

ATOMIC, MOLECULAR, OPTICS – THEORY

CLUSTERS

DYNAMICS

FEL SOURCES & SCIENCE

VUV SOURCES & SCIENCE

CONDENSED MATTER – EXPERIMENTAL

CONDENSED MATTER – THEORY

HIGH ENERGY X-RAY PHOTOELECTRON SPECTROSCOPY

INSTRUMENTATION

MICROSCOPY

ATOMIC, MOLECULAR, OPTICS – EXPERIMENTAL

5P001 **Cassia Turci**

Ionic decay of core excited states and fragmentation dynamics of aromatic molecules

5P002 **Christopher Chantler**

Accurate measurement and physical insight: The X-ray extended range technique for fundamental atomic physics, condensed matter research and biological sciences

5P003 **Zheng Wei**

Mapping both direct and core-resonant double photoemission from the Cu (001) surface

5P004 **C. Y. Robert Wu**

High resolution fluorescence spectrometry: the N₂ emissions

5P005 **David Holland**

The effect of autoionization on very low energy photoelectron angular distributions and vibrational/rotational populations

5P006 **Minna Patanen**

High resolution study of K 3p photoabsorption and resonant Auger decay in KF

5P007 **Wenzheng Fang**

The photoionization study of several mono-terpenes in the region 7.8 eV – 16.0 eV

5P008 **Arathi Padmanabhan**

A dissociative photoionization study of the c⁴Σ_u⁻ state in O₂⁺ using the TPEPICO technique

5P009 **James Harries**

Lifetime-resolved H⁺ fluorescence following O 1s excitation / ionisation in gas-phase water molecules

5P010 **Oksana Travnikova**

Influence of the circular polarized light on the electronic relaxation and nuclear dynamics of the core-excited states of SF₆ at the F 1s edge

5P011 **Alexandre Lago**

Cationic and anionic photodissociation of thionyl chloride following deep-core level excitation

5P012 **Hirokichi Niikura**

Measuring attosecond molecular electron wavepacket motion by controlling re-colliding electron pulses

5P013 **Antti Kivimäki**

Photoabsorption, photoionization and photoelectron – Auger electron coincidence studies of the SF₆ molecule at and above the S 2p edge

5P014 **Kiyoshi Ueda**

Angle-resolved rescattering-electron spectra of O₂ and CO₂ molecules induced by ultra-short intense laser pulses

5P015 **Kiyoshi Ueda**

Sequential three-photon double ionization of Ar atoms irradiated by EUV-FEL at SPring-8

5P016 **Thomas Gerber**

Dissociative photoionization of energy-selected CH₃I⁺: iPEPICO at SLS/VUV beamline

5P017 **Kuno Kooser**

Resonant Auger electron-ion coincidence study of the fragmentation dynamics of acrylonitrile molecule

- 5P018 **Shin-ichi Wada**
Anionic dissociation of methyl-ester thin films induced by inner-shell excitations
- 5P019 **Kazumichi Nakagawa**
Oscillator strength distribution of DNA bases from 3 to 250 eV
- 5P020 **Michael Kolbe**
Coster-Kronig probabilities and fluorescence yields of high Z elements determined experimentally with a reliable uncertainty budget
- 5P021 **Darrah Thomas**
Recoil-induced rotational excitation in the valence ionization of CO and N₂
- 5P022 **Jun-ichi Adachi**
C 1s photoelectron angular distributions from fixed-in-space CO₂ and OCS molecules with kinetic energy above 50 eV
- 5P023 **Flavio Rodrigues**
Electronic excitation and ionic dissociation of core-excited sulfur compounds related with the ocean-atmosphere cycle: DMS and DMDS
- 5P024 **Markus Fieß**
Isolated attosecond laser pulses tunable between 80 and 100 eV
- 5P025 **Dang Trinh Ha**
Ab initio and ion-ion coincidence study on the dissociation of d-ribose molecules
- 5P026 **Dennis Lindle**
Three-membered heterocyclic molecules by partial ion yield spectroscopy: C₂H₄O and C₂H₄S
- 5P027 **Brenton Lewis**
Extreme-ultraviolet Fourier-transform spectroscopy of N₂ and CO
- 5P028 **Piotr Forsysinski**
PFI-ZEKE photoelectron spectrum of CH₂F₂ from the adiabatic ionization potential to the onset of fragmentation
- 5P029 **John Neville**
Double ionisation and ionic fragmentation of the isomers propyne and allene
- 5P030 **Uwe Becker**
Two-centre interference effects in valence photoelectron emission of N₂ and O₂
- 5P031 **Minna Patanen**
Atom - solid binding energy shifts for K and Rb
- 5P032 **Hiroaki Yoshida**
Coulomb explosion dynamics of multiply ionized CF₄
- 5P033 **Sébastien de Rossi**
Optical metrology of multilayer mirrors for attosecond light pulse
- 5P034 **Charles Bourassin-Bouchet**
Spatio-temporal manipulation of attosecond pulses with mirrors
- 5P035 **Yudai Izumi**
Soft X-ray natural circular dichroism of aspartic acid and tyrosine
- 5P036 **Ralph Püttner**
Probing molecular dications with Auger spectroscopy
- 5P037 **Jérôme Palaudoux**
Double Auger decay of 1s holes in CO, CO₂ and O₂
- 5P038 **Ana Mónica Ferreira-Rodrigues**
UV and X-ray excitation and fragmentation of nitriles by EELS and TOF-MS
- 5P039 **Eero Itälä**
Site selective fragmentation of pyrimidine derivatives
- 5P040 **Jérôme Palaudoux**
HBr³⁺ states populated after Br 3d ionization
- 5P041 **Jérôme Palaudoux**
Multielectron coincidence spectroscopy of mercury vapor
- 5P042 **Kueih-Tzu Lu**
State-specific enhanced production of positive ions and negative ions of gaseous SiCl₄ and solid-state analogues following core-level excitation

5P - THURSDAY, JULY 15, 16:10-18:00 *continued*

- 5P043 **Victor Kimberg**
Core-excited wave packet dynamics beyond the Born-Oppenheimer approximation studied by angle-resolved resonant Auger scattering in O₂
- 5P044 **Giovanni Stefani**
Plasmon decay mechanism studied by e-e coincidence experiment
- 5P045 **Grazieli Simões**
Core-level photoabsorption, photoionization and gas emission in sulfur-containing biomolecules subjected to ionizing radiation
- 5P046 **Dennis Lindle**
Nondipole photoemission from chiral enantiomers of camphor
- 5P047 **Uwe Becker**
Direct observation of fullerene plasmon oscillations in momentum space
- 5P048 **Frank Filsinger**
Target preparation for diffractive X-ray imaging of gas-phase molecules
- 5P049 **Yuhai Jiang**
XUV pump-probe visualizing ultrafast isomerization of Acetylene-Vinylidene cations at FLASH
- 5P050 **Thomas Gerber**
iPEPICO studies on atmospherically relevant S_xO_yCl_z ions

ATOMIC, MOLECULAR, OPTICS - THEORY

- 5P051 **Christopher Chantler**
Ab initio determination of K_α line strengths, energies and spectator intensities in transition metal atoms
- 5P052 **Wenzheng Fang**
A VUV photoionization organic aerosol mass spectrometric study with synchrotron radiation
- 5P053 **Ming-Hui Shang**
Photoemission from valence bands of transition metal-phthalocyanine
- 5P054 **Johannes Niskanen**
Valence photoionization of LiCl monomer and dimer

- 5P055 **Johannes Niskanen**
Photoelectron angular distribution and linear magnetic dichroism in the 4p photoemission from Rb atoms
- 5P056 **Pascal Quinet**
Atomic data for VUV lines of astrophysical interest in singly ionized rhodium
- 5P057 **Jérôme Palaudoux**
Manifestation of PCI in cascade double Auger decay of Ar 2p holes
- 5P058 **Andrey Pavlychev**
Vibrational and rotational excitations associated with inner-shell ionization in small molecules
- 5P059 **Zhili Wang**
Efficiency of the extraction algorithm in grating-based X-ray phase imaging
- 5P060 **Andrey Pavlychev**
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5P001

Ionic decay of core excited states and fragmentation dynamics of aromatic molecules

ALF Barros,¹ R Paschoal,¹ AC Guerra,¹ G Ferreira,² C Turci²¹Centro Federal de Educação Tecnológica- CEFET-RJ, Rio de Janeiro, Brazil; ²Universidade Federal do Rio de Janeiro- UFRJ, Rio de Janeiro, Brazil

Inner-shell excitation and associated decay spectroscopies are site specific probes of electronic and geometrical structure and photoionization dynamics. X-ray absorption probes the geometric and electronic structure, while time-of-flight mass spectrometry with multi-coincidence detection provides information on the photofragmentation dynamics of the initially produced inner-shell state. Auger decay of inner-shell excited and ionized states is an efficient source of multiply charged ions. We wish to study ionic fragmentation following core excitation of a series of aromatic gas phase molecules, using the time-of-flight multi-ion coincidence apparatus. Although our group has particular interest in the isomeric nitroanilines, known as *push-pull* system, here we present the K-edge coincidence studies of gaseous benzene, aniline, nitrobenzene, toluene and chlorobenzene, that are the fundamental importance to understand the *push-pull* system. The ionic fragmentation has been measured with tuned synchrotron light and time-of-flight mass spectrometry apparatus. Our goal is to investigate the fragmentation dynamics of those aromatic molecules aiming to answer the following question: How the both donor and acceptor groups influencing the charge transfer into the aromatic ring and, consequently, their fragmentation dynamics? The experiments have been performed using the Spherical Grating Monochromator (SGM) beamline at the National Laboratory of Synchrotron Light (LNLS) in Campinas-SP, Brazil (research proposals D08A-SGM-7250 and 8730).

5P002

Accurate measurement and physical insight: the X-ray extended range technique for fundamental atomic physics, condensed matter research and biological sciences

CT Chantler¹¹School of Physics, university of Melbourne, Parkville, Victoria, Australia

Research in core physics and atomic and condensed matter science are increasingly relevant for diverse fields and are finding application in chemistry, engineering and biological sciences, linking to experimental research at synchrotrons, reactors and specialized facilities. Over recent synchrotron experiments and publications we have developed methods for measuring the absorption coefficient far from the edge and in the XAFS (X-ray absorption fine structure) region in neutral atoms, simple compounds and organometallics reaching accuracies of below 0.02%. This is 50–500 times more accurate than earlier methods, and 50–250 times more accurate than claimed uncertainties in theoretical computations for these systems. The data and methodology are useful for a wide range of applications, including major synchrotron and laboratory techniques relating to fine structure, near-edge analysis and standard crystallography. Experiments are sensitive to theoretical and computational issues, including correlation between convergence of electronic and atomic orbitals and wavefunctions. Hence, particularly in relation to the popular techniques of XAFS and XANES (X-ray absorption near-edge structure), this development calls for strong theoretical involvement but has great applications in solid state structural determination, catalysis and enzyme environments, active centres of biomolecules and organometallics, phase changes and fluorescence investigations and others.

[1] J. L. Glover et al., Phys. Rev. A 78 (2008) 052902

[2] N. A. Rae et al., Phys. Rev. A 81 (2010) 022904

[3] M. T. Islam et al., Phys. Rev. A 81 (2010) 022903

5P003

Mapping both direct and core-resonant double photoemission from the Cu (001) surface

Z Wei,¹ G van Riessen,¹ RS Dhaka,¹ C Winkler,¹ FO Schumann,¹ J Kirschner¹¹Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We have studied the emission of electron pairs upon the absorption of a single photon. The measurements were performed with a set-up which consists of two hemispherical analyzers which were operated at the BESSY II storage ring. The light polarization was linear and we selected a photon energy which was far above the 3p threshold. This energy selection allows us to investigate the double photoemission process from valence electrons (direct channel) in parallel to the excitation of a core photoelectron and subsequent emission of an Auger electron (core-resonant channel). As expected for a single-step process mediated by electron correlation, the two electrons emitted by the direct channel continuously share the energy available to them. The core-resonant channel is often considered in terms of successive and independent steps of photo-excitation and Auger decay. In this case one expects the energy sharing to be defined by the kinetic energy of photoelectron and Auger electron. However, this expectation is at odds with our experimental evidence. We find that electron pairs emitted by the core-resonant channel also share their energy continuously to jointly conserve the energy of the complete process. By detecting the electron pairs in parallel over a wide range of energy, evidence of the core-resonant double photoemission proceeding by a coherent single-step process is most strikingly manifested by a continuum of correlated electron pairs with a sum energy characteristic of the process but for which the individual electrons have arbitrary energies and cannot meaningfully be distinguished as a photoelectron or Auger electron.

5P004

High resolution fluorescence spectrometry: the N₂ emissionsCYR Wu,¹ JI Lo,² YC Lin,² YJ Chen,² TS Yih,² HS Fung,³ YY Lee,³ DL Judge¹¹University of Southern California, Los Angeles, CA, United States; ²National Central University, Jhongli, Taiwan; ³National Synchrotron Radiation Research Center, Hsinchu, Taiwan

We have studied the strongly coupled $c_4'(0)$ and $b'(1)$ states and the $b(1)$ state of N₂. We have found that the $c_4'(0)$ state predominantly decays through resonance fluorescence to the ground state while the $b'(1)$ state prefers the $b'(1)-a$ branching transition and the subsequent cascade $a-X$ (LBH) emissions. Our preliminary results also indicate that the branching ratio for $[b(1)-a]/[b(1)-X]$ is much higher than that based on the factor of the transition frequency ratio alone, which only amounts to 0.01. We are currently carrying out similar experiments on N₂ at temperatures as low as 77 K so that the data can be directly applicable to the characterization of the N₂ emissions in the atmospheres of Titan and Pluto. Detailed results will be presented.

5P005

The effect of autoionization on very low energy photoelectron angular distributions and vibrational/rotational populationsDMP Holland,¹ DA Shaw¹¹Photon Science Department, Daresbury Laboratory, Warrington, Cheshire, Great Britain

A velocity map imaging spectrometer, incorporating a delay-line detector, has been constructed to allow the velocity distributions of electrons or ions, formed through photoionization, to be measured. The spectrometer design is based upon the original configuration described by Eppink and Parker, but also includes a double Einzel lens to enhance the collection efficiency of energetic particles, together with two pairs of deflectors to enable the image to be centred on the detector. Results are shown to illustrate the use of this spectrometer to study electronic autoionization in molecular nitrogen and vibrational autoionization in molecular hydrogen. In both molecules, images have been recorded as the excitation energy is scanned across a resonant state, and the influence of autoionization upon the photoelectron angular distributions is readily observed. These changes in the velocity distributions are particularly evident for electrons possessing very low kinetic energies. Vibrational autoionization in molecular hydrogen significantly affects both the photoelectron angular distributions and rotational populations. Although individual rotational levels cannot be resolved, the rotational population distributions exhibit variations, with autoionization tending to enhance the population of low rotational levels. The observed photoelectron angular distributions and vibrational/rotational populations are compared with theoretical predictions. The spectrometer has also been employed to study dissociative photoionization in molecular oxygen and images of the fragment ion angular distributions demonstrate alignment effects.

5P006

High resolution study of K 3p photoabsorption and resonant Auger decay in KFM Patanen,¹ S Urpelainen,² M Huttula,¹ V Kisand,³ E Nõmmiste,³ E Kukkk,⁴ H Aksela,¹ S Aksela¹¹Department of Physics, University of Oulu, Oulu, Finland; ²Max-lab, Lund University, Lund, Sweden; ³Institute of Physics, University of Tartu, Tartu, Estonia; ⁴Department of Physics, University of Turku, Turku, Finland

Tunable and monochromatized high-intensity synchrotron radiation facilities have offered enormous possibilities to study specific excited states of molecules, and to select, not only the electronic, but also the vibronic state. Resonant Auger (RA) spectroscopy is an excellent tool for studying nuclear dynamics and electronic decay of excited molecular states. In this study we have used RA spectroscopy to study the $K3p\sigma/\pi \rightarrow K4s \uparrow$ excitation in molecular KF. This excitation decays via participator RA transition. The resonance states were mapped in the photon energy range of 18.2-19.4eV recording total ion yield (TIY) spectrum, and the RA spectra were measured at the highest resonances. Spectra were measured at the FINEST branch on the I3 beamline on MAX-III storage ring in MAX-lab, Sweden. The emitted Auger electrons were recorded using the Scienta SES-100 electron analyzer and ions with TOF-spectrometer. The experimental spectra are interpreted using non-relativistic *ab initio* molecular calculations corrected with perturbation theory treatment for spin-orbit interaction. The RA simulations took the life-time vibrational interference into account. Molecular calculations for the electronic states were performed using the GAMESS code. The simulated photoabsorption and RA spectra were found to agree well with the experimental TIY and RA spectra. The structure of the RA spectra reflects the different nodal structures of the wavefunctions at different vibrational levels in the excited electronic state. The time scales of the nuclear relaxation and the electronic decay are of the same order of magnitude, so the electronic decay has high probability to take place before the vibrational wavepacket reaches its second turning point. This study demonstrates the potential of the FINEST branchline when high resolution is needed, e.g. in studies of the vibrational structure in molecular spectra.

5P007

The photoionization study of several mono-terpenes in the region 7.8~16.0 eVL Gong,¹ W Fang,¹ X Shan,¹ F Liu,¹ Z Wang,² L Sheng¹¹School of Nuclear Science and Technology, National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui, China;²Laboratory of Environmental Spectroscopy, Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui, China

The photoionization of three characteristic mono-terpenes (R-[+] limonene, S-[+] carvone, L-menthone) has been studied for the first time in the region 7.8~16.0 eV, using tunable VUV synchrotron radiation and time-of-flight mass spectrometry. The adiabatic ionization energies of them were derived from experiment and found to be 8.27, 8.78 and 8.70 eV which compared well with B3LYP calculations yielding results of 8.14, 8.51 and 8.61 eV [6-311++G]. The appearance energies of their major fragment ions were observed with photoionization efficiency spectra. The base peak m/z 68 [C⁵H₈⁺] in the mass spectra of limonene above 13.0 eV referred to as an isoprene unit resulting from a retro Diels-Alder reaction has a significant activation energy. Interestingly, the R-DA reaction also occurs in the fragmentation of carvone with the products of 2-Methyl-but-1,3-dien-1-one (m/z 82) ion and isoprene (m/z 68) above 11.0 eV.

5P008

A dissociative photoionization study of the c⁴Σ_u⁻ state in O₂⁺ using the TPEPICO technique.A Padmanabhan,¹ M MacDonald,² C Ryan,² L Zuin,² TJ Reddish¹¹Physics Department, University of Windsor, Windsor, ON,, Canada; ²Canadian Light Source, Saskatoon, SK, Canada

We have investigated the angular distributions of 2 eV O⁺ following dissociative photoionization from the c⁴Σ_u⁻ state in O₂⁺ for both v = 0 and 1 by measuring the coincidence yield between threshold photoelectrons and angle- and energy-resolved photoions. The experiments were performed using a toroidal spectrometer [1] in conjunction with linearly polarized synchrotron radiation on the VLS-PGM (undulator) beamline at the Canadian Light Source. We determined the *ratio* of the v = 0, 1 photoion angular distributions from which one can, in principle, study the lifetimes of these levels. The different dissociation lifetimes smear-out the 'inherent' anisotropic photoion angular distribution, characterized by a β parameter. Our results show that the inherent β value for the c⁴Σ_u⁻ state is 0.41 ± 0.08, giving rise to measurable β values of 0.3 and 0.1 for the v = 1 and 0 levels, respectively, once lifetime effects are considered. These values are in general agreement to the observed β values of 0.35 and 0.0 [2] and at variance with the theoretical inherent β value of 1.6 [3]. How these β values contribute to the ongoing discussion on the lifetimes will be presented at the conference, along with the details of the experimental method.

[1] Reddish *et al*, Rev Sci Instrum **68** 2685 [1997][2] Lafosse *et al* J Chem Phys **117** 8368 [2002][3] Lin and Lucchese, J Chem Phys **116** 8863 [2002]

5P009

Lifetime-resolved H* fluorescence following O 1s excitation / ionisation in gas-phase water moleculesJR Harries,¹ T Gejo,² JP Sullivan,³ Y Azuma⁴¹Japan Atomic Energy Agency, SPring-8, Japan; ²University of Hyogo, Hyogo, Japan; ³Australian National University, Canberra, Australia; ⁴Sophia University, Tokyo, Japan

Photo-excitation/ionisation of the O 1s electron in gas-phase water molecules can produce neutral, excited hydrogen atoms following Auger decay and dissociation. The excited (or ionised near-threshold) electron acts as a spectator as the excited H₂O⁺ core undergoes Auger decay, leading to a fast ejected electron and a two-hole, H₂O²⁺ ion. The ion dissociates, and one of the outgoing fragments can capture the initially excited electron. When this fragment is a proton, a neutral H atom is formed, and if this is in an excited state, the fluorescence can be observed as it decays. Previous studies [e.g. PRL **96**, 063003 (2006)] have analysed this fluorescence in the energy domain. Here we resolve the fluorescence in the time domain, which allows H* states of higher n and specific l to be identified. Beamline 27SU at SPring-8 was used, and Lyman-α photons were counted as a function of incident photon energy. The arrival times of the photons were determined with respect to the pulses of incident radiation. The decay profiles were fitted to continuous lifetime distributions, in a new application of the lifetime-resolved fluorescence spectroscopy technique [J.Phys.B **36**, L319(2003)].

5P010

Influence of the circular polarized light on the electronic relaxation and nuclear dynamics of the core-excited states of SF₆ at the F1s edge

O Travnikova,¹ JC Liu,² A Lindblad,¹ C Nicolas,¹ J Söderström,¹ V Kimberg,¹ F Gel'mukhanov,² C Miron¹

¹Synchrotron SOLEIL, Saint-Aubin, France; ²Department of Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden

High resolution electron spectroscopy of highly symmetric molecules surrounded by strongly negative ligands such as e.g. SF₆, CF₄ has drawn a lot of interest in a recent decade. F1s⁻¹ Auger atomic-like decay following F1s → a_{1g}* core-excitation induced by the linear polarized light has been observed. In these studies it has been shown that the F1s⁻¹ core-hole localization and bond elongation along the polarization vector is preferred, which leads to the ultrafast dissociation on the timescale of the F1s core hole lifetime (~2 fs) and the consequent observation of the Doppler-split atomic lines in the direction parallel to the polarization vector. In this study the effect of the circular polarized light in comparison to the linear polarized light on the nuclear dynamics of F1s → a_{1g}* core-excited SF₆ is investigated. We present the experimental evidence for the occurrence of an Auger-Doppler effect following inner-shell excitation by circularly polarized X-rays when their frequency is tuned on top of the F1s → a_{1g}* transition in SF₆. The measurements were performed at the new ultra high resolution soft X-ray beamline PLEIADES at SOLEIL synchrotron radiation facility in France. [1] M. Kitajima, Phys. Rev. Lett. **91**, 213003 (2003), [2] G. Prümper, J. Phys. B **31**, 1 (2005) [3] K. Ueda, Phys. Rev. Lett. **90**, 233006 (2003).

5P011

Cationic and anionic photodissociation of thionyl chloride following deep-core level excitation

AF Lago,¹ JZ Dávalos,² WC Stolte,³ IN Demchenko⁴

¹Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André - SP, Brazil; ²Instituto de Química-Física "Rocasolano", CSIC, Madrid, Spain; ³Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, USA; ⁴Department of Chemistry, University of Nevada, Las Vegas, USA

The photo-fragmentation of the thionyl chloride (SOCl₂) molecule has been investigated near the Chlorine and Sulfur K edges using ion yield spectroscopy. Total and partial ion yield and mass spectra have been recorded as function of the photon energy. The experiments were performed with the use of synchrotron radiation from the 9.3.1 beamline of the Advanced Light Source and a 180° magnetic mass spectrometer. Several singly and multiply charged ions have been identified, including the following anions (Cl⁻, O⁻, S⁻). Interesting differences in the ion yield spectra for the anions have been observed as one move from the sulfur to the chlorine K edge, and those are discussed in a comparative way. The spectra are dominated by atomic singly and multiply-charged fragments. The fragmentation processes were governed by complex decay mechanisms involving singly and multiply charged species formed below and above the ionization threshold, as well as via dissociation into ion pairs. Fragmentation pathways have been proposed from the analysis of the spectra. This work provides the first experimental report of negative ion formation from the dissociative photoionization of thionyl chloride molecule following excitation in the vicinity of the S and Cl K shells. This work was financially supported by FAPESP and CNPq (Brasil), Ministerio de Educación, Cultura y Deporte (Spain) and U.S. Department of Energy.

5P012

Measuring attosecond molecular electron wavepacket motion by controlling re-colliding electron pulses

H Niikura,^{1,2,4} H Wöner,² D Villeneuve,² P Corkum^{2,3}

¹Department of Applied Physics, Waseda University, Tokyo, Japan; ²National Research Council, Ottawa, Canada; ³Department of Physics, University of Ottawa, Ottawa, Canada; ⁴PRESTO, Japan Science and Technology Agency, Tokyo, Japan

High harmonics is generated during ionization of atoms or molecules under intense laser fields. A spectrum of high harmonics contains information on their vibration, electronic structure, and electron dynamics. Using orthogonally polarized two-color laser pulses, we demonstrate that electron motion in a molecule can be mapped onto high harmonic generation spectra with attosecond time-resolution. To identify electron motion, we measure the relationship between the polarization angle (Φ_{HHG}) of the high harmonics and the electron re-collision angle (θ_c). Φ_{HHG} depends on both θ_c and a spatial distribution of a bound state electron wavefunction. If amplitude and phase of the electron wavepacket changes dynamically after tunnel ionization, then Φ_{HHG} follows its motion. We overlap 400 nm and 800 nm intense laser pulses and generate high harmonics from a target molecule without alignment. We control the re-colliding electron trajectory and thus θ_c by changing the relative delay between the two laser pulses. For non-aligned molecules, high harmonics is preferentially generated from that portion of the ensemble which dominates the ionization probability. It allows us to probe an electron wavefunction with π_g symmetry. We measure the spectra as a function of the relative delay between the two laser pulses. First, we identify symmetry of the electron wavefunction which is mostly responsible for high harmonic generation process for N₂, CO₂, and N₂O. Next, we measure electron wavepacket motion in a polyatomic molecule which is prepared by intense field ionization in the range from 1.3 to 1.7 fs.

5P013

Photoabsorption, photoionization and photoelectron – Auger electron coincidence studies of the SF₆ molecule at and above the S 2p edge

A Kivimäki,¹ L Avaldi,² P Bolognesi,² M Coreno,² P O'Keeffe,² V Feyer,³ J Alvarez Ruiz,⁴ M Stankiewicz,⁵ M Stener,⁶ G Fronzoni,⁶ P Decleva⁶
¹CNR-IOM, TASC Laboratory, Trieste, Italy; ²CNR-IMIP, Monterotondo Scalo, Italy; ³Sincrotrone Trieste, Trieste, Italy; ⁴IOFR-CSIC, Madrid, Spain; ⁵Uniwersytet Jagiello ski, Krakow, Poland; ⁶Università di Trieste, Trieste, Italy

Electronic transitions involving the S 2p orbitals of the SF₆ molecule have been studied experimentally and theoretically. The S 2p photoabsorption spectrum of SF₆ was measured with a windowless double ionization cell and calculated using time dependent density functional theory, whereby spin orbit coupling for bound transitions is included. The main features of the experimental spectrum – intense excitations to the virtual valence orbitals (with anomalous intensity ratios for the spin-orbit components) and weak Rydberg excitations – are well reproduced by the calculations. For the region above the S 2p edge, our theoretical approach gives properly the positions of the 2t_{2g} and 4e_g shape resonances and predicts at higher photon energies EXAFS oscillations, which are also visible in the photoabsorption spectrum. The S 2p photoelectron spectra were measured over an extended photon energy range, from below the 4e_g shape resonance to above the S 2s edge. The intensities of the spin-orbit-resolved S 2p lines display oscillating behaviors in the photon energy range 205-230 eV, in agreement with theory, and a strong Fano-type resonance at the S 2s → 6t_{1u} excitation. Via an electron-electron coincidence experiment, we have also decomposed the Auger spectrum measured at the S 2p → 4e_g shape resonance into the components deriving from the S 2p_{3/2} and S 2p_{1/2} hole states and from the shake-up satellite state.

5P014

Angle-resolved rescattering-electron spectra of O₂ and CO₂ molecules induced by ultra-short intense laser pulses

M Okunishi,¹ H Niikura,^{1,2,3} T Morishita,^{3,4} R Lucchese,^{1,5} K Ueda¹

¹IMRAM, Tohoku Univ., Sendai, Miyagi, Japan; ²Dep. of Appl. Phys., Waseda Univ., Tokyo, Japan; ³PRESTO, Kawaguchi, Saitam, Japan; ⁴Dep. of Appl. Phys. and Chem., Univ. of Electro-Communications, Chofu, Tokyo, Japan; ⁵Dep. of Chem., Texas A&M Univ., College Station, Texas, United States

Angle resolved high-energy rescattering-electron spectra of randomly oriented O₂ and CO₂ molecules are measured with near-IR laser pulses in the range of laser intensities from 7x10¹³W/cm² to 1.2x10¹⁵W/cm². At the lowest laser intensity, we use 100 fs laser pulse. For larger laser intensities, we use shorter pulse duration (35fs and 10fs) in order to reduce electron saturation on the ionization. High-energy electrons that are rescattered by their parent ions are detected with a linear TOF spectrometer as a function of the angle between the laser (linear) polarization and the direction of emission of the electrons. Using a procedure proposed by Chen *et al* [1], we extract differential cross sections (DCS) for elastic electron-ion scattering from the 2D rescattering electron spectra as a function of collision momentum (p=0.9-3.2 a.u.). Suppression of the DCS for the backward direction at around p=1 and 3 (a.u.) is observed for both molecules and we can explain it by the destructive interference of the electron scattering waves coming from the two O atoms for O₂ and from the C and O atoms for CO₂. A theoretical analysis of the DCS to extract the structural information of the molecule is in progress.

[1] Z. Chen, *et al*, J. Phys. B: At. Mol. Opt. Phys. 42, 061001 (2009)

5P015

Sequential three-photon double ionization of Ar atoms irradiated by EUV-FEL at SPring-8

H Fukuzawa,^{1,2} EV Gryzlova,^{1,2,3} K Motomura,^{1,2} A Yamada,^{1,2} K Ueda,^{1,2} AN Grum-Grzhimailo,³ SI Strakhova,³ K Nagaya,^{2,4} A Sugishima,^{2,4} Y Mizoguchi,^{2,4} H Iwayama,^{2,4} M Yao,^{2,4} N Saito,^{2,5} P Piseri,^{1,2,6,7} T Mazza,^{1,2,6,7} M Devetta,^{1,2,6,7} M Coreno,^{2,8} M Nagasono,² K Tono,² M Yabashi,² T Ishikawa,² H Ohashi,^{2,9} H Kimura,^{2,9} T Togashi,^{2,9} Y Senba⁹

¹IMRAM, Tohoku University, Sendai, Japan; ²RIKEN XFEL, Sayo, Japan; ³Inst. of Nucl. Phys., Moscow State University, Moscow, Russian Federation; ⁴Dept. of Phys., Kyoto University, Kyoto, Japan; ⁵NMIJ, AIST, Tsukuba, Japan; ⁶Università di Milano, Milano, Italy; ⁷CIMAINA, Milano, Italy; ⁸CNR-IMIP, Montelibretti (Roma), Italy; ⁹JASRI, Sayo, Japan

We have investigated sequential three-photon double ionization (STPDI) of Ar atoms by extreme ultraviolet (EUV) free-electron laser (FEL) pulses from SPring-8 Compact SASE Source (SCSS) test accelerator [1] by means of electron spectroscopy. The SCSS test accelerator provides linearly polarized EUV-FEL pulses. The photon energy was set to 24 eV, which is enough to ionize neutral Ar atom but not enough to ionize Ar⁺(3p⁵) ion. We have observed the photoelectron lines corresponding to the STPDI with resonantly enhanced two-photon ionization of the Ar⁺(3p⁵) via the intermediate Ar⁺(3p⁴n) even states. The relative intensities of the photoelectron peaks and their angular dependence have been explained in the framework of a three-step model of the process.

We are grateful to the SCSS Test Accelerator Operation Group at RIKEN for continuous support in the course of the studies.

[1] T. Shintake *et al.*, Nature Photonics 2, 555 (2008).

5P016

Dissociative photoionization of energy-selected CH_3I^+ : iPEPICO at SLS/VUV beamline

T Gerber,¹ A Boedi,¹ NS Shuman,² T Baer,² B Szta³ ray³

¹Paul Scherrer Institut, Villigen, Switzerland; ²University of North Carolina, Chapel Hill, NC, United States; ³University of the Pacific, Stockton, CA, United States

The dissociative photoionization onset energy of the $\text{CH}_3\text{I} \rightarrow \text{CH}_3^+ + \text{I}$ reaction was studied at the VUV beamline of the Swiss Light Source (SLS) with a new imaging photoelectron photoion coincidence (iPEPICO) apparatus. A photon energy resolution of 2 meV and a threshold electron kinetic energy resolution of ≈ 1 meV were achieved. Three previous attempts at establishing this value accurately, namely a pulsed field ionization (PFI)-PEPICO measurement, *ab initio* calculations and a mass analyzed threshold ionization (MATI) experiment, in which the onset energy was bracketed by state-selected excitation to vibrationally excited $^2\text{A}_g$ states of the parent ion, have yielded contradictory results. It is shown that dimers and adducts formed in the supersonic molecular beam affected the PFI-PEPICO onset energy. The room temperature iPEPICO experiment yields an accurate 0 K onset of 12.248 ± 0.003 eV, from which we derive a $\Delta fH_{298\text{K}}^\circ(\text{CH}_3\text{I}) = 15.4 \pm 0.3$ kJ mol⁻¹.

5P017

Resonant Auger electron-ion coincidence study of the fragmentation dynamics of acrylonitrile molecule

K Kooser,^{1,2} DT Ha,¹ E Itälä,¹ S Granroth,¹ L Partanen,³ A Caló,³ S Aksela,³ H Aksela,³ E Nömmiste,² E Kukk¹

¹University of Turku, Turku, Finland; ²University of Tartu, Tartu, Estonia; ³University of Oulu, Oulu, Finland

Acrylonitrile may be regarded as a derivate of ethylene ($\text{CH}_2=\text{CH}_2$) by substituting one of the hydrogen atoms with the cyano group ($\text{C}=\text{N}$). This molecule is considered to be an important industrial chemical. On the other hand acrylonitrile plays an important role in astrochemistry, while this molecule and its fragments caused by cosmic radiation are present in interstellar medium. Here we present the investigation results of the photodissociation and possible geometrical rearrangements of acrylonitrile molecule induced by the core level electron excitations of the cyano group atoms and discussed depending on the character of the preceding electronic relaxation channels and/or the kinetic energy of ejected Auger (or photo-)electrons. The comparison of the electron-ion coincidence maps of the $\text{N } 1s^{-1}\pi^*$ and $\text{C } 1s^{-1}\pi^*$ Auger decay shows that the fragmentation channels are the same and the energy dependency on the initial site of core hole creation is very weak. However, the main features of these coincidence maps strongly depend on the final cationic state reached by Auger decay of the core excited states. The acrylonitrile fragmentation pathways depending on the nature of resonant decay channel and concerning the possible migration of light H atoms during the excitation and after that have been discussed and the existence of metastable states of acrylonitrile fragments have been reported.

5P018

Anionic dissociation of methyl-ester thin films induced by inner-shell excitations

S Wada,^{1,2} A Hirano,¹ K Yufu,¹ H Ishida,¹ K Tanaka³

¹Department of Physical Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ³RIKEN SPring-8, Sayo-gun, Hyogo, Japan

Production of negatively charged ions by inner-shell excitations is interesting phenomenon because the excited states necessarily decay via positive ionic states. In this study, we investigated anionic dissociation/desorption reactions following inner-shell excitations of PMMA thin films ($-\text{[CH}_2\text{C(CH}_3\text{)COOCH}_3\text{]}_n-$) and methyl-ester terminated self-assembled monolayers (MHDA- d_3 SAMs; Au-S(CH_2)₁₅COOCD₃). Experiments were performed at the beamlines BL-13 of HiSOR, Hiroshima University and BL7A of KEK PF. Desorbing negative ions from photoirradiated samples were measured by means of a conventional TOF-MS with an additional magnetic field to prevent electrons to the detector. Atomic negative fragments, H⁻, D⁻ and O⁻, were detected by C and O K-edge excitations. The shape of yield spectrum of H⁻ ion resembles that of the TEY spectrum. So, it can be considered that dominant H⁻ fragments are produced by dissociative electron attachment by Auger and secondary electrons. On the other hand, spectrum of D⁻ indicates increase in the yield at excitations to the $\sigma^*(\text{O-CD}_3)$ and C-H*/Rydberg states. The $\sigma^*(\text{O-CD}_3)$ excitation causes site-selective O-CD₃ bond breaking via spectator-type Auger decay [1]. Such Auger final states can preferentially produce not only CD₃⁺ ion but also CD₃^{*} neutral fragments. When an initially core-excited electron remains around a D site in CD₃^{*}, CD₃^{*} dissociates via ion-pair formation of D⁻ and CD₂⁺. Enhancement of D⁻ fragmentation at the Rydberg state can be also explained by the similar mechanism with recapture of the Rydberg electron. [1] S. Wada et al., J. Phys.: Condens. Matter. 18, S1629 (2006).

5P019

Oscillator strength distribution of DNA bases from 3 to 250 eVKR Koswattage,¹ A Mimoto,¹ Y Izumi,¹ A Imazu,¹ M Tanaka,¹ M Tanabe,¹ K Nakagawa¹¹Graduate School of Human Development and Environment, Kobe University, Kobe, Japan

Oscillator strength distribution of molecules within wide energy range is very important and fundamental data for not only basic molecular science but also for application such as radiation effect induced by high energy photons or high energy particles. We measured absolute values of oscillator strength distribution of DNA bases (guanine, thymine, cytosine and adenine), from 3 to 250 eV using synchrotron radiation. Thin films of DNA base molecules were prepared with the vacuum sublimation technique around 370 K of heating temperature on the collodion films supported on stainless steel mesh. Thickness of the film was roughly estimated by a quartz oscillator thickness monitor to be around 30 nm. Precise values of thickness were determined by comparison of absorption strength measured by a commercial ultraviolet spectrometer with the spectra measured with synchrotron radiation. Optical absorption spectra from 3 to 250 eV were measured at beamlines 5B and 7B of the UVSOR synchrotron radiation facility in the Institute for Molecular Science, Okazaki, Japan. Accuracy of absolute values of oscillator strength was examined with the Thomas-Reihe-Kuhn sum rule. For the case of guanine, thymine, cytosine and adenine, we obtained values of integrated oscillator strength from 3 to 250 eV to be 58, 47, 43 and 44, respectively. These values should be equal to the number of total electrons associating to optical transition from 3 to 250 eV, 56, 48, 42 and 50, for guanine, thymine, cytosine and adenine, respectively. Only for adenine, difference of 12% was observed, of which reason is not clear at the present time. Characteristics of radiation damage induced by radiation will be discussed on the basis of obtained absorption spectra.

5P020

Coster-Kronig probabilities and fluorescence yields of high Z elements determined experimentally with a reliable uncertainty budgetM Kolbe,¹ M Müller,¹ B Beckhoff¹¹Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany

A further methodological development for the determination of L-subshell atomic fundamental parameters by pure photon-in-photon-out experiments will be presented. At the electron storage ring BESSY II Coster-Kronig probabilities and fluorescence yields of high Z elements have been experimentally determined. Thin foils of these elements have been investigated with monochromatized synchrotron radiation of high spectral purity and well-known flux employing calibrated instrumentation of PTB. Hence, all experimental parameters are well known including their relative uncertainties. The intensities of the fluorescence lines have been determined for different photon energies for selective excitation of the three L-subshells. The transmittance of the self-supporting one-elemental foils employed has been determined in order to derive self-absorption correction factors depending on the photon energy of both the exciting and the fluorescence radiation. This ensured a traceable uncertainty budget for the determined fundamental parameters. The knowledge of all experimental, instrumental and fundamental parameters involved, enables XRS to be used as a reference free analytical method [1], which is needed especially for the characterisation of advanced materials.

[1] Beckhoff, J. Anal. At. Spectrom. 23, 845-853 (2008)

5P021

Recoil-induced rotational excitation in the valence ionization of CO and N₂TD Thomas,¹ K Ueda,² E Kukk,³ LJ Sæthre⁴

¹Department of Chemistry, Oregon State University, Corvallis, OR, United States; ²Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan; ³Department of Physics, University of Turku, Turku, Finland; ⁴Department of Chemistry, University of Bergen, Bergen, Norway

Recoil-induced rotational excitation accompanying photoionization has been measured for the X, A, and B states of N₂ and CO over a range of photon energies from 60 eV to 900 eV. The mean recoil excitation increases linearly with the kinetic energy of the photoelectron, with slopes ranging from 0.73×10^{-5} to 1.40×10^{-5} . These slopes are generally in accord with a simple model that takes into account the atom from which the electron is emitted, the molecular-frame angular distribution of the electron, and the dependence of the photoelectron cross section on photon energy, on atomic identity, and on the type of atomic orbital from which the electron is ejected. These measurements thus provide a tool for investigating the atomic-orbital composition of the molecular orbitals. Additional insight into this composition is obtained from the relative intensities of the various photolines in the spectrum and their variation with photon energy. A quantum-mechanical treatment of recoil-induced excitation predicts an oscillatory variation with photon energy of the excitation. However, the predicted oscillations are small compared with the uncertainties in the data, and, as a result, the currently available results cannot provide confirmation of the quantum-mechanical theory.

5P022

C 1s photoelectron angular distributions from fixed-in-space CO₂ and OCS molecules with kinetic energy of above 50 eV

J Adachi,¹ M Kazama,² N Miyauchi,¹ M Yamazaki,³ T Fujikawa,² A Yagishita¹

¹Photon Factory, IMSS, KEK, Tsukuba, Japan; ²Graduate School of Integrated Science, Chiba Univ., Chiba, Japan; ³IMRAM, Tohoku Univ., Sendai, Japan

Photoelectron diffraction phenomena have been used to determine material structures, in particular, for the surfaces, the interfaces, and the adsorbed molecules. However, conventional measurement techniques cannot be applied to free molecules because of thermal molecular rotation. Investigating the electron scattering phenomenon as a fundamental quantum process requires measurement without any effects from the substrates or surrounding environment. Recently, we improved the coincidence velocity-map imaging spectrometer to measure molecular-frame photoelectron angular distributions (MFPADs) with kinetic energy (KE) of above 50 eV, which opens a study on the elementary process of low-kinetic energy photoelectron diffraction for free molecules. We measured MFPADs from carbon 1s levels of CO₂ and OCS molecules from $KE \sim 50$ to ~ 150 eV. The present results may be considered as the observation of low-energy photoelectron diffraction patterns involving modulations in extended X-ray absorption fine structure spectra. Simulation calculations with the multiple scattering theory will be performed to intuitively explain the origins of the MFPAD patterns.

5P023

Electronic excitation and ionic dissociation of core-excited sulfur compounds related with the ocean-atmosphere cycle: DMS and DMDS

R Bernini,¹ L da Silva,² F Rodrigues,¹ L Coutinho,³ G G de Souza²

¹Instituto Federal do Rio de Janeiro, Rio de Janeiro, RJ, Brazil; ²Instituto de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ, Brazil; ³Centro Universitário Educacional da Zona Oeste, Rio de Janeiro, RJ, Brazil

The natural flux of sulfur to the atmosphere occurs mainly through volatile sulfur compounds (known as reduced sulfur compounds) produced in oceans. It is believed that the earth's climate can be influenced by these reduced sulfur compounds through modification of the radiation budget. In the present work, photoabsorption and ionic fragmentation spectra were obtained for the dimethyl sulfide (DMS) and dimethyl disulfide (DMDS) molecules excited around the S 2p edge, using synchrotron radiation. DMDS can also be seen as a prototype for the study of the role of disulfide bridges (-S-S- bonds) in molecules. Mass spectra, using a time of flight spectrometer, were recorded for both molecules at different energies, around the resonances observed in the S 2p photoabsorption spectra. Extensive fragmentation occurs at the core level energy-range. Double ionization is clearly observed in the two molecules. Interestingly, both the S⁺ (DMS) and S₂⁺ (DMDS) cations show a significant enhancement in intensity at the S 2p $\tau 0$ virtual states resonances, pointing out to a possible site-selective fragmentation. For the sake of comparison, valence-shell mass spectra were obtained for these molecules (19 eV photon energy). Extensive fragmentation occurs at the core level. For example, at 185 eV photon energy, the dominant fragments are H⁺ and CH₃⁺. Double ionization of the molecule is clearly demonstrated with the observation of the S²⁺ fragment ion. Similar electron impact excitation and ionic fragmentation studies of these molecules are currently under development in our laboratory. The authors acknowledge CNPQ, FAPERJ and LNLS (Brazil) for financial assistance.

5P024

Isolated attosecond laser pulses tunable between 80 and 100 eV

M Fieß,¹ M Schultze,^{1,4} B Horvath,² M Hofstetter,^{1,4} W Helml,¹ Y Cheng,³ B Zeng,³ Z Xu,³ A Scrinzi,⁴ J Gagnon,¹ R Kienberger,^{1,5} F Krausz^{1,4}

¹Max-Planck-Institute of Quantum Optics, Garching, Germany; ²ABB Corporate Research Center, Baden-Daettwil, Switzerland; ³State Key Laboratory of High Field Laser Physics, Shanghai, China; ⁴Ludwig-Maximilians-Universität München, Munich, Germany; ⁵Technische Universität München, Munich, Germany

We report on the generation of isolated attosecond laser pulses tunable in the spectral range between 80 and 100 eV which are generated by high harmonic generation in Ne-gas with driving laser pulses and its second harmonic. We present XUV spectra for different fundamental waveforms which are synthesized by controlling the phase delay between the driving laser field and its second harmonic wave. Furthermore we present a novel interferometer setup for attosecond pump-probe experiments based on metal coated mirrors which support XUV spectra between 70 and 130 eV. Photoelectron streaking measurements with attosecond laser pulses as broad as 30 eV, which have been generated by conventional high harmonic generation with the fundamental driving laser field, demonstrate the reliability of the interferometer setup. Finally we give an outlook for a combination of tunable attosecond laser pulses with the presented interferometer setup for flexible attosecond pump-probe experiments.

5P025

Ab initio and ion-ion coincidence study on the dissociation of d-ribose moleculesDT Ha,^{1,2} M Huels,^{3,4} M Huttula,⁵ S Urpelainen,⁵ E Kukkk¹

¹Dept. of Physics and Astronomy, University of Turku, Turku, Finland; ²Graduate School of Materials Research, Turku, Finland; ³Royal Institute of Technology KTH, Atomic and Molecular Physics, Stockholm, Sweden; ⁴Dept. of Nuclear Medicine and Radiology, Faculty of Medicine, University of Sherbrooke, Sherbrooke, Quebec, Canada; ⁵Dept. of Physical Sciences, University of Oulu, Oulu, Finland

As a continuation of our recent series of studies on damage to DNA components by soft X-rays, we have recently investigated similar damage to DNA/RNA sugars. The PEPIICO (PhotoElectron-Photon-Photon Coincidence) method was used to record the photodissociation of doubly charged d-ribose ($C_5H_{10}O_5$) molecules which are the result of initial C 1s core ionization, followed by normal Auger decay. High resolution photoelectron spectra were recorded in coincidence with time of flight mass spectra. The measurement instrument consists of a modified Scienta SES-100 hemispherical electron analyzer and a Wiley-McLaren type ion time-of-flight spectrometer. The experiments were carried out at the undulator beamline I411 at the MAX-II storage ring. Our main purpose is to study the dissociation channels of doubly ionized molecules following core-ionization by using synchrotron radiation. This is an essential step in attempting to understand radiation damage to DNA components in nature by the very lethal low energy, or soft X-rays. In addition, the GAMESS software was used to perform *ab initio* calculations to model the dissociation processes. Properties such as appearance energies, equilibrium and intermediate states of the conformations of the molecules and their dissociated fragments were examined in order to outline the dissociating dynamics.

5P026

Three-membered heterocyclic molecules by partial ion yield spectroscopy: C_2H_4O and C_2H_4S WC Stolte,¹ I Dumitriu,² SW Yu,³ G Ohrwall,⁴ MN Piancastelli,⁵ DW Lindle¹

¹Chemistry Department, University of Nevada Las Vegas, Las Vegas NV, United States; ²Physics Department, Western Michigan University, Kalamazoo, MI, United States; ³Lawrence Livermore National Laboratory, Livermore, CA, United States; ⁴MAX-lab, Lund University, Lund, Sweden; ⁵Department of Physics and Material Science, Uppsala University, Uppsala, Sweden

We have investigated the photo-fragmentation properties of two three-membered ring heterocyclic molecules, C_2H_4O and C_2H_4S , by total and partial ion yield spectroscopy. Positive and negative ions have been collected as a function of photon energy around the C 1s and O 1s ionization thresholds in C_2H_4O , and around the S 1s and 2p edges and the C 1s threshold for C_2H_4S . We underline some similarities and differences between these two analogous systems.

5P027

Extreme-ultraviolet Fourier-transform spectroscopy of N_2 and COAN Heays,¹ G Stark,² BR Lewis,¹ JR Lyons,³ PL Smith,⁴ N de Oliveira⁵

¹Australian National University, ACT, Australia; ²Wellesley College, MA, United States; ³University of California, CA, United States; ⁴Harvard-Smithsonian Center for Astrophysics, MA, United States; ⁵Synchrotron Soleil, St. Aubin, France

New N_2 and CO photoabsorption measurements have been made employing the Fourier-transform spectrometer on the DESIRS beamline of the SOLEIL synchrotron. Measurement in the extreme-ultraviolet energy range is made possible by a unique window- and beam-splitter-free interferometer, employing wavefront division in a Fresnel configuration. The maximum achievable resolution at 100 nm is 0.00016 nm and a simultaneous measurement is made over the undulator bandpass of approximately 5 nm. Spectra have been obtained for nitrogen between 89 nm and 79.4 nm at resolutions as fine as 0.00023 nm, and various column densities. Measurements of CO spectra have been obtained between 119 nm and 90 nm for the isotopomers $^{12}C^{16}O$, $^{13}C^{16}O$, $^{12}C^{17}O$, and $^{13}C^{18}O$. Because of the narrow and well-characterized instrument profile of the Fourier-transform spectrometer, these measurements are suitable for the determination of predissociation linewidths and relative f values for individual rotational lines. These f values will be fixed to an absolute scale following comparison with previous measurements. The inherently accurate wavelength calibration also enables the confident determination of all transition energies. Immediate application of these spectra lies in the modelling of photolysis in an astrophysical context [1]. Also, this data will support the development of quantum-mechanical models of molecular photoabsorption and photodissociation at the Australian National University.

1. Liang *et al.* (2007), *Astrophys. J.*, 664:L115-L118.

5P028

PFI-ZEKE photoelectron spectrum of CH_2F_2 from the adiabatic ionization potential to the onset of fragmentation

PW Forsyński,¹ P Zielke,¹ D Luckhaus,¹ R Signorell¹

¹Chemistry Department, UBC, Vancouver, BC, Canada

The first vibrationally resolved pulsed-field-ionization zero-kinetic-energy (PFI-ZEKE) photoelectron spectrum of difluoromethane from its adiabatic ionization potential to the onset of the first ionic fragmentation channel is presented.* Measurements are recorded on a recently reported†, newly set-up photoelectron/photoion spectrometer for the investigation of the interaction of extreme ultraviolet (EUV) light (wavelength $\geq 70\text{nm}$) with molecules, clusters and aerosol particles. PFI-ZEKE spectroscopic studies of the difluoromethane monomer are performed as a stepping stone on the way to larger systems. Precise values for the adiabatic ionization potential and the appearance potentials of the H loss product and the F loss product of the cation are reported. *Ab initio* harmonic and 9D anharmonic calculations are performed in an attempt to assign the newly observed vibrational structure which, in its previously published low resolution form, led to numerous speculations regarding its true origin. Anharmonic effects are shown to be extremely important in the shallow potential of the difluoromethane cation‡, and calculations with corrections up to the CCSD(T)/aug-cc-pVQZ level of theory show very good agreement with experiment.

* Forsyński *et al.*, *Phys. Chem. Chem. Phys.*, 2010, **12**, 3121.

† Zielke *et al.*, *J. Chem. Phys.*, 2009, **130**, 211101.

‡ Luckhaus *et al.*, *Mol. Phys.*, 2010, in press.

5P029

Double ionisation and ionic fragmentation of the isomers propyne and allene

JJ Neville,¹ R Igarashi,² A Sankari,³ R Sankari,² L Zuin²

¹Department of Chemistry, University of New Brunswick, Fredericton, NB, Canada; ²Canadian Light Source Inc., Saskatoon, SK, Canada; ³Department of Synchrotron Radiation Research, Lund University, Lund, Sweden

Propyne and allene are two of the three stable isomers of C_3H_4 . They are significant in combustion and soot fragmentation processes and are also of astrophysical significance, having been identified for example in comets and the atmosphere of Titan. In a previous C 1s excitation study of propyne, we have observed molecular rearrangement processes accompanying ionic fragmentation, in particular a hydrogen atom shift from the methyl carbon to either of the triply bonded carbons. Other studies of the photolysis and isomerisation of propyne and allene following ultraviolet excitation suggest that conversion between the two occurs readily with lower-energy excitation, although isomeric differences persist even as the excitation energy increases. In the present study, the dissociative double ionisation of propyne and allene following vacuum ultraviolet absorption near the double ionisation thresholds has been investigated. High brightness, narrow bandwidth synchrotron radiation from the VLS-PGM beamline at the Canadian Light Source has been used in combination with ion time-of-flight mass spectrometry and photoelectron-photoion-photoion coincidence (PEPIICO) techniques to obtain photoionisation branching ratios and ion-pair branching ratios. The stability of the lowest-energy dicationic states of the target molecules has been investigated, providing insight to the role of the initial structure and electronic configuration in the stabilisation of the dication and the dynamics following double ionisation.

5P030

Two-centre interference effects in valence photoelectron emission of N_2 and O_2

M Braune,¹ M Ilchen,² S Korica,¹ A Meißner,¹ L Tribedi,¹ S Deinert,² L Glaser,² F Scholz,² P Walter,² J Viefhaus,² U Becker^{1,3}

¹FHI der MPG, Berlin, Germany; ²DESY, Hamburg, Germany; ³KSU, Riyadh, Saudi Arabia

In the photoionization of homonuclear diatomic molecules interference effects occur due to the fact that the photoelectron emission sites are indistinguishable. As a consequence periodic intensity variations appear in the photoionization cross sections with increasing photon energy. This topic was addressed by Cohen and Fano in their famous paper [1] and interferences of this kind are referred to as Cohen-Fano oscillations ever since. The oscillatory behavior in the valence photoionization of N_2 and O_2 which they presented as experimental evidence, however, turned out to be basically an intensity variation due to a shape resonance rather than a signature of coherent emission from two emitter sites. The oscillation period of a real Cohen-Fano type oscillation depends on the internuclear distance and extends over a broad energy range as has been proven many years later for the 1s core photoionization of H_2 and N_2 . According to recent calculations for nitrogen [2] reflections of the Cohen-Fano oscillations should also arise in the angular distribution of photoelectron emission. We present corresponding data for the outer valence photoionization of N_2 and O_2 as a result of our most recent angular resolved photoelectron spectroscopy experiments. Derived values for the dipole anisotropy parameters and cross section ratios corroborate indeed an oscillation with a period proportional to the inverse bond length, as predicted by Cohen and Fano.

[1] H.D. Cohen and U. Fano, *Phys. Rev.* **150**, 30 (1966)

[2] D. Toffoli, P. Decleva, *J. Phys. B* **39**, 2681 (2006)

5P031

Atom - solid binding energy shifts for K and RbM Holappa,¹ S Aksela,¹ M Patanen,¹ S Urpelainen,² H Aksela¹¹Department of Physics, University of Oulu, Oulu, Finland; ²MAX-lab, Lund University, Lund, Sweden

Binding energy shifts between free atoms and solids are very important in electron spectroscopy. Values of binding energy shifts from vapor to solid are not accurate if the vapor is measured with respect to vacuum and solid with respect to Fermi level due to inaccuracies in the determination of work function. The determination of work function can be avoided if the vapor and solid measurements are done simultaneously so the both are respect to vacuum level. The experiments were carried out at the undulator beamline I411 at the 1.5 GeV MAX-II storage ring in MAX-lab, Sweden. In our measurements a cool needle like surface was located into the vapor beam and the spectra from the vapor around the tip and from the condensed solid layer were detected simultaneously. Using this experimental setup both vapor and solid state spectra could be observed simultaneously in identical experimental conditions. In this study 2p photolines of K and 3d photolines of Rb for atom and solid are measured and the binding energy shifts between atom and solid are reported. These samples are interesting because for K 2p and Rb 3d photolines no simultaneous measurements for vapor and solid have been reported previously. Alkali metal clusters are widely studied and our measurements can be used as a reference for clusters studies.

5P032

Coulomb explosion dynamics of multiply ionized CF₄H Yoshida,^{1,2} Y Kimura,¹ I Miyagami,¹ A Hiraya^{1,2}¹Department of Physical Science, Hiroshima University, Higashi-Hiroshima, Japan; ²Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan

Multiply-charged ion is often produced by inner-shell ionization through Auger decay and it generally dissociates into some fragment ions by Coulomb explosion. We have investigated the dissociation dynamics of inner-shell ionized CF₄. Experiments were carried out on the soft X-ray beamline BL-6 at the synchrotron radiation facility HiSOR in Hiroshima University. A time-of-flight mass analyzer equipped with a two-dimensional position-sensitive detector (RoentDek DLD-40) was used to obtain the initial momenta of emitted ions created by Coulomb explosion. Angular and energy distributions of ejected ions are obtained measuring three-dimensional initial momenta derived from detected positions (X, Y) and flight times (T) of fragment ions. Distributions of correlation angles for θ_1 ($F_{(first\ hit)}^+$, $F_{(second\ hit)}^+$), θ_2 ($F_{(first\ hit)}^+$, CF^+), and θ_3 ($F_{(second\ hit)}^+$, CF^+) in the (F^+ , F^+ , CF^+) formation process after C1s ionization of CF₄ are obtained. Both θ_2 and θ_3 distribute $\sim 120^\circ$. The F-C-F angle in the stable structure of the neutral ground state is 109.5° with T_d symmetry. The experimental value of $\sim 120^\circ$ is larger than it. On the other hand, θ_1 distributes $\sim 113^\circ$, which is relatively close to 109.5° . The simultaneous 4-body dissociation process ($CF_4^{4++} \rightarrow F^+ + F^+ + CF^+ + F$) is considered to estimate the momentum of undetected neutral fragment 'F' using the following equation: $\mathbf{P}_F = -(\mathbf{P}_{F_1} + \mathbf{P}_{F_2} + \mathbf{P}_{CF^+})$. The calculated correlation angles for (F, F⁺) and (F, CF⁺) using the experimental results are 100° and 97° , respectively. Total kinetic energy release in the present Coulomb explosion process including the kinetic energy of undetected neutral fragment 'F' is estimated to be 21.8 eV.

5P033

Optical metrology of multilayer mirrors for attosecond light pulseS de Rossi,¹ C Bourassin-Bouchet,¹ F Delmotte,¹ E Meltchakov,¹ Z Diveki,² D Guenet,² T Ruchon,² P Salières,² B Carré,² A Giglia,³ N Mahne,³ S Nanaronne³¹Laboratoire Charles Fabry, Institut d'Optique, Univ. Paris Sud, CNRS, RD 128 Campus Polytechnique, Palaiseau, France; ²CEA-Saclay, IRAMIS, Service des Photons, Atomes et Molécule, Gif-sur-Yvette, France; ³Laboratorio TASC-INFN-CN, Trieste, Italy

Doing physics with attosecond pulses requires efficient broadband optical systems with a well controlled phase. In the extreme ultraviolet the only efficient solution to work with light is the multilayer mirror. For this purpose we have optimized three aperiodic mirrors with three different optical functions: a 40 eV broadband mirror working near normal incidence; a 20 eV broadband mirror with linear phase working at 45° incidence; a 20 eV broadband mirror with parabolic spectral phase working at 45° incidence. All multilayers have been deposited using a magnetron sputtering system. We have performed our metrology measurements on synchrotron source. The measurement of the module of the reflectivity is common. For the determination of the phase, we have measured the photo-electrons emitted at the top of the multilayer. We have also measured our mirrors by using a high order harmonics source. The complex reflectivity of the stacks have been obtained thank to the RABBIT technique. This method is a direct access to the spectral phase unlike the photoelectron measurements. In both case we compare the experimental performances with the simulations. This full optical characterization is a way to understand the effect of the multilayer structure on attosecond pulses and achieve in the future new optical functions such as an attosecond pulseshaper.

5P034

Spatio-temporal manipulation of attosecond pulses with mirrors**C Bourassin-Bouchet,¹ S de Rossi,¹ F Delmotte,¹ P Chavel,¹ Z Diveki,² D Guenot,² T Ruchon,² P Salières,² B Carré²**¹Laboratoire Charles Fabry, Institut d'Optique, Univ Paris sud, CNRS, RD128 Campus Polytechnique, Palaiseau, France; ²CEA-Saclay, IRAMIS, Service des Photons, Atomes et Molécules, Gif-sur-Yvette, France

Attosecond light pulses (1 as = 10^{-18} s) can nowadays be produced by high-harmonic generation in the Extreme Ultraviolet (EUV). In this spectral range, the best way to manipulate and/or focus such pulses is based on multilayer mirrors which efficiently reflect EUV radiation. In order to properly manipulate attosecond pulses, the spectral response of such optics, set by the multilayer stack, has to be optimized. In particular, the spectral phase should be carefully controlled over the full spectral bandwidth. We designed and manufactured three plane multilayer mirrors with optimized reflectivity and spectral phase in the 20eV-70eV range near 45° incidence. Their spectral response has been fully characterized on the Elettra Synchrotron and on an attosecond pulse source at CEA SPAM. A combination of two mirrors with a suitable filter may provide with an active attosecond pulse-shaper. It allows the realization of some simple functions as an accordable pulse compression, or the shaping of a single, double or multiple sub-100 as pulses, the properties of which can be set by simply turning the pulse-shaper. Moreover focusing attosecond pulses is essential for numerous applications. But current focusing mirrors can be aberrating, which leads to strong spatio-temporal distortions of the attosecond pulses. This results in a loss of their attosecond structure, as shown by numerical studies. Consequently, in addition to the multilayer structure, the shape of the focusing mirror has to be carefully chosen. This leads to a spatio-temporal pulseshaping, where both wavefront and spectral phase are controlled during the reflexion of pulses on the mirror.

5P035

Soft X-ray natural circular dichroism of aspartic acid and tyrosine**Y Izumi,¹ M Tanabe,¹ A Imazu,¹ A Mimoto,¹ K Nakagawa,¹ M Tanaka,² A Agui,³ T Muro⁴**¹Graduate School of Human Development and Environment, Kobe University, Hyogo, Japan; ²National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan;³Japan Atomic Energy Agency, Hyogo, Japan; ⁴Japan Synchrotron Radiation Research Institute, Hyogo, Japan

We measured soft X-ray natural circular dichroism (SXNCD) of aspartic acid (Asp) and tyrosine (Tyr) at oxygen K-edge region, in an attempt to obtain chiral structure at the vicinity of oxygen atoms. SXNCD measurement was carried out at the BL25SU beamline of the SPring-8, Japan. We focused on oxygen $\text{COO}^- 1s \rightarrow \pi^*$ transitions around 533 eV. Since we used sublimation films which are randomly oriented samples, we could reject E1E2 mechanism and pick up only E1M1 mechanism. It is well known that nonequivalent oxygen atoms in COO^- group, which is common part of amino acids, give two components. For L-Asp and L-Tyr, negative and positive SXNCD peaks were observed in this work at lower and higher energy side, respectively. This result is quite different from previous results in which for L-Ser with positive and negative peaks and for L-Ala with only one negative peak were reported [Izumi et al., 2009]. Although theoretical studies by three groups are partly available, unified understanding is not achieved yet. Co-works between experimental and theoretical studies will be inevitable.

5P036

Probing molecular dications with Auger spectroscopy**R Püttner,¹ V Sekushin,¹ T Arion,² M Förstel,² T Lischke,² M Mucke,² H Fukuzawa,³ K Ueda,³ T Asahina,⁴ N Kuze,⁴ H Kato,⁴ M Hoshino,⁴ H Tanaka,⁴ G Kaindl,¹ TD Thomas,⁵ E Kukk,⁶ AM Bradshaw,² U Hergenhahn²**¹FU Berlin, Berlin, Germany; ²Max-Planck-Institut für Plasmaphysik, Garching, Germany; ³Tohoku University, Sendai, Japan; ⁴Sophia University, Tokyo, Japan; ⁵Oregon State University, Corvallis, USA; ⁶University of Turku, Turku, Finland

Auger spectroscopy is a powerful tool for studying molecular dications, M^{2+} . In the case of metastable dicationic species the Auger spectrum resulting from the creation of a shallow core hole displays spectral features with vibrational fine structure. This allows a Franck-Condon analysis of the vibrationally resolved Auger spectrum to be performed and, by including in a sophisticated fit analysis the lifetime interference terms, one can obtain from such spectra detailed information about the potential energy curves of the metastable dicationic states. As an example of such studies we will present recent results obtained for NO. The Auger spectra of *dissociative* dicationic species, however, consist of broad features which are difficult to analyze. By employing a new high-resolution experimental setup to measure photoelectron and Auger electron spectra in coincidence we were able to separate the $\text{C } 1s^{-1} v=0$ and $v=1$ Auger spectra of CH_4^{2+} . These spectra display pronounced differences due to the fact that the energy spectrum of a transition to a dissociative state reflects the squares of the vibrational wavefunction, $\Psi_{\text{vib}}^2(Q)$, in the singly core-ionized state. By implementing this in a simultaneous fit of both spectra we have separated the Auger transitions to all 7 states of dicationic CH_4^{2+} present in this energy region. We were able to derive the energy values and slopes of the potential energy curves of the dicationic states and have found good agreement with other experimental and theoretical results. Results for fluorine-containing molecules, which also involve dissociative states, will be discussed.

5P037

Double Auger decay of 1s holes in CO, CO₂ and O₂**J Palaudoux,^{1,2} L Andric,^{1,2,3} P Lablanquie,^{1,2} F Penent,^{1,2} K Bucar,⁴ M Zitnik,⁴ M Huttula,⁵ K Ito,⁶ JHD Eland⁷**¹LCP-MR, Université Pierre et Marie Curie, Paris, France; ²CNRS, Paris, France; ³Université Paris-Est, Marne-la-Vallée, France; ⁴Jožef Stefan Institute, Ljubljana, Lithuania;⁵Department of Physical Sciences, Oulu, Finland; ⁶Photon Factory, Tsukuba, Japan; ⁷Physical and Theoretical Chemistry Laboratory, Oxford, Great Britain

The emission of two Auger electrons, associated with the decay of 1s holes in CO, CO₂ and O₂ molecules has been investigated experimentally with synchrotron light produced at SOLEIL (TEMPO beam line). The HERMES experiment consists in a magnetic bottle time of flight spectrometer coupled with a light chopper used to increase the light pulse intervals from the synchrotron, operated in single bunch mode. This results in a high energy resolution and high electron detection efficiency, suitable for coincidence experiments, as demonstrated in previous studies on double Auger decays in Ar, Xe and CS₂. The Double Auger (DA) decays were characterized by analyzing in energy the three electrons of the process, detected in coincidence: the 1s photoelectron and the two Auger electrons. DA decays associated with C1s and O1s holes in CO and CO₂, as well as with both O 1s⁻⁴ ²Σ and ⁴Σ states in O₂ were separated. We observe a weak 'direct' DA path in which the 2 Auger electrons are emitted simultaneously with a continuous energy sharing, and a dominating cascade one in which an intermediate AB⁺⁺ is produced. One observes also that this intermediate state can dissociate fully into (A⁺, B⁺) fragments prior to the emission of the second Auger electron, which is then an atomic fragment coming from autoionization of the B⁺⁺ fragment.

5P038

UV and X-ray excitation and fragmentation of nitriles by EELS and TOF-MS**AM Ferreira-Rodrigues,^{1,4} FN Rodrigues,^{2,4} HM Boechat-Roberty,³ GGB de Souza⁴**¹Natural Science Department - Federal University of the State of Rio de Janeiro (UNIRIO), Rio de Janeiro/RJ, Brazil; ²Physics Department - Federal Institute of Rio de Janeiro (IFRJ), Rio de Janeiro/RJ, Brazil; ³Valongo Observatory - Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro/RJ, Brazil; ⁴Physical-Chemistry Department - Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro/RJ, Brazil

Nitriles like acetonitrile (CH₃CN) and acrylonitrile (CH₂CHCN) are present in planetary and cometary atmospheres and in interstellar medium, in star forming regions. Newly formed stars emit electrons, UV and X-ray photons which dissociate nitriles into reactive fragments. These fragments may participate in the formation of more complex molecules such as amino acids. In this work, we have studied the electronic excitation of these molecules, in the valence region (4 – 48 eV), using the electron energy loss spectroscopy technique with high resolution and with angular variation (1.5° to 6°) and low resolution in the range of 0 to 200 eV. Photoabsorption cross section and the corresponding oscillator strength were obtained for the first time, in this entire region. New transitions have been observed and have been assigned to Rydberg series. With the scattering spectrum, in the less angle, were determined the polarizability and the elastic cross section in a range of 1.5° to 50°. The Bethe surface to 1.5°, 2.0°, 3.0°, 4.0°, 5.0° and 6.0° scattering angles of acetonitrile were obtained. The core ionization and fragmentation of the acetonitrile and acrylonitrile molecules was studied using synchrotron radiation and time of flight mass spectroscopy technique, for the 210 – 310 eV region. Partial ion yields, photodissociation and photoionization cross sections and the survival ratio for these molecules was determined. This work contributes to explain the photoabsorption and destruction of these molecules in star forming region.

5P039

Site selective fragmentation of pyrimidine derivatives**E Itälä,¹ DT Ha,¹ K Kooser,¹ E Rachlew,² MA Huels,³ E Nõmmiste,⁴ U Joost,⁴ E Kukkk¹**¹University of Turku, Turku, Finland; ²Royal Institute of Technology, KTH, Stockholm, Sweden; ³University of Sherbrooke, Sherbrooke, QC, Canada;⁴University of Tartu, Tartu, Estonia

By tuning the photon energy to a desired transition, one can core-ionize a certain atom in a complex molecule and possibly expect a selective breakage of the surrounding bonds. The breakage is preceded by Auger decay, rate of which depends on the overlap between the core hole orbital and the molecular orbitals involved in the Auger process. As the molecule becomes more complex, the number of different fragmentation channels increases and the probability of strong site selective fragmentation decreases. Despite of this, the site selective fragmentation in three pyrimidine derivatives; thymine, uracil and 5-bromouracil is studied here. The experimental method used here is electron energy resolved photoelectron-photoion-photoion coincidence spectroscopy (PEPICO), which allows the investigation of ion fragments as a function of the initial ionization site (C 1s). The different ionization sites are visible in the photoelectron spectrum as individual peaks, because the carbon atoms in the pyrimidine ring are in different chemical environments, which causes the splitting of the photolines. The site selectivity appears as deviations in coincident ion pair intensities when moving from lower binding energy to higher indigo energy. In order to consider the possible factors effecting on site selectivity, the results of each sample are compared without forgetting the fragmentation differences between the samples in general.

5P040

HBr³⁺ states populated after Br 3d ionizationJ Palaudoux,^{1,2} F Penent,^{1,2} L Andric,^{1,2,3} G Gamblin,^{1,2} P Lablanquie,^{1,2} K Ito,⁴ JHD Eland,⁵ S Carniato^{1,2}¹LCP-MR, Université Pierre et Marie Curie, Paris, France; ²CNRS, Paris, France; ³Université Paris-Est, Marne-la-Vallée, France; ⁴Photon Factory, Tsukuba, Japan; ⁵Physical and Theoretical Chemistry Laboratory, Oxford, Great Britain

We present here results on HBr triple ionization resulting from Double Auger (DA) decay after Br 3d inner-shell ionization. Experiments were performed at BESSY synchrotron operated in single bunch mode (with a mechanical chopper that extends the light period to 12 μs), using a magnetic bottle time of flight spectrometer (HERMES) that allows coincident detection of all the electrons. The detection of the 3d photoelectron with 2 Auger electrons emitted simultaneously allow to identify a weak 'direct' DA decay to HBr³⁺ states in the Frank Condon region. However, the dominant DA decay channel results from cascade with a 1st Auger decay to an HBr²⁺ intermediate state that can dissociate into [H⁺, Br²⁺] fragments prior to the emission of a 2nd Auger electron which results from autoionization of the Br⁺ fragment. The identification of Br⁺[Br²⁺(²D)]n Rydberg series decaying to Br²⁺ ⁴S lead us to revise the Br²⁺ ²D_{5/2} : ²D_{3/2} spin orbit splitting. *Ab initio* MCSCF calculations depict the lowest HBr³⁺ electronic states involved in direct DA process, up to their dissociation limits and reveal their peculiar topology resulting from the dominating Coulomb repulsion in the [H⁺, Br²⁺] system combined with a residual binding of the [H, Br³⁺] system.

5P041

Multielectron coincidence spectroscopy of mercury vaporJ Palaudoux,^{1,2} M Huttula,³ SM Huttula,³ L Andric,^{1,2,4} P Lablanquie,^{1,2} F Penent^{1,2}¹LCP-MR, Paris, France; ²CNRS, Paris, France; ³Department of Physical Sciences, Oulu, Finland; ⁴Université Paris-Est, Marne-la-Vallée, France

Electron spectroscopy is a well established method for studies of electronic structure of matter in all its forms. Presently, third generation synchrotron radiation (SR) sources and multi electron coincidence setups are common tools for experimentalists. The magnetic bottle time-of-flight (MB-TOF) spectrometer developed by J Eland for multielectron coincidence spectroscopy has been implemented for use with synchrotron radiation to study photon induced multielectron transitions in rare gas atoms and small molecules. Electron coincidence studies following core ionization of metal atoms by synchrotron radiation are still rare. Here, we present studies on the electronic transitions in mercury vapor ([Xe]4f¹⁴5d¹⁰6s²). The experiments were carried out at U 125/2 beamline at the Bessy-II synchrotron in Berlin, Germany. The MB-TOF spectrometer was coupled to a multi-hit TDC to measure electron time of flight. Coincidences between n electrons allow us to observe the populations of Hgⁿ⁺ final states, and particularly to establish the yet unknown spectroscopy of Hg³⁺ and Hg⁴⁺ ions. Coincidences reveal also the main mechanisms leading to their formation, by the observation of the Auger decay channels of the spin-orbit splitted 4f and 5p core holes states. Weaker processes such as population and decay of photoionization satellites and core-valence double ionization are also characterized. Relativistic Multiconfiguration Dirac Fock calculations have been used to predict the spectral features in good agreement with the experimental findings.

5P042

State-specific enhanced production of positive ions and negative ions of gaseous SiCl₄ and solid-state analogues following core-level excitationKT Lu,¹ JM Chen,¹ JM Lee,¹ SC Haw,¹ YC Liang¹¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan

The state-specific dissociation dynamics of ionic (positive ion and negative ion) and excited neutral fragments of gaseous SiCl₄ and SiCl₄ adsorbed on Si(100) ~90 K following Cl 2p core-level excitations were investigated on combining measurements of photon-induced ion dissociation, X-ray absorption, and UV/visible dispersed fluorescence. The Cl⁺ desorption yield shows a significant enhancement following Cl 2p → 8a₁⁺ excitation of condensed SiCl₄, while Cl 2p core-level excitation of gaseous SiCl₄ leads to the scarce enhancement of the Cl⁺ yield. In contrast, the Cl 2p → 9t₂⁺ and Cl 2p → Rydberg excitations of gaseous SiCl₄ lead to a notable enhancement in the Si⁺ yield, as compared to the Cl 2p → 8a₁⁺ excitation. Excitations of the Cl 2p electrons to Rydberg orbitals near the Cl 2p ionization threshold of gaseous SiCl₄ lead to a remarkably enhanced production of anionic, Si⁻ and Cl⁻ fragments and excited neutral atomic, Si^{*}, fragments. The enhanced production of anionic and excited neutral fragments via core-level excitation near the ionization threshold of gaseous SiCl₄ is explained in terms of the contributions from the shake-modified resonant Auger decay or/and post-collision interaction (PCI). The anionic Cl⁻ yield of SiCl₄/Si(100) with variable coverage up to 35 L was measured via Cl 2p core-level excitation. The Cl 2p → 8a₁⁺ excitation of SiCl₄/Si(100) leads to a notable enhancement in the Cl⁻ yield, particularly for lower coverage. These complementary results provide new insight into the state-selective ionic and excited neutral fragmentation processes of gaseous molecules and solid-state analogs via core-level excitation.

5P043

Core-excited wave packet dynamics beyond the Born-Oppenheimer approximation studied by angle-resolved resonant Auger scattering in O₂

V Kimberg,¹ A Lindblad,¹ O Travnikova,¹ J Soderstrom,¹ C Nicolas,¹ C Miron¹

¹Synchrotron SOLEIL, Gif-sur-Yvette, France

The Born-Oppenheimer (BO) or adiabatic approximation breaks down near the crossings of the diabatic potential energy curves. Quite often, the non-BO behaviour is observed in the processes related to excitation and de-excitation of the core electrons, when the vibronic coupling between electronic configurations results in nontrivial nuclear dynamics in the core-excited state. A puzzling feature observed in the X-ray absorption spectrum of oxygen molecule near 539 eV that arises from the Rydberg-valence mixing. This feature got much attention and was studied extensively both in experiment and theory [1]. With the help of numerical simulations, it was shown recently, that explicit consideration of all interchannel couplings between the Rydberg and the valence manifolds allows to explain in detail the formation of the X-ray absorption spectra near the O1s → σ* resonance in O₂ [2]. In the present paper, we make another attempt to study the nuclear dynamics in the core-excited state with the help of high resolution resonant Auger spectroscopy (RAS). Our angle-resolved measurements, together with theoretical simulations, allow detailed discussing of the RAS vibrational profile, resulting from interplay of resonant and direct ionization channels, as well as from the dynamics of the coupled wave packet in the core-excited state.

[1] R. Feifel, *et al.*, J. Chem. Phys. **128**, 064304 (2008); [2] Y. Velkov, *et al.*, Chem. Phys. Lett. **476**, 147 (2009)

5P044

Plasmon decay mechanism studied by e-e coincidence experiment

A Ruocco,¹ WSM Werner,² Ml Trioni,³ F Offi,¹ S Iacobucci,⁴ W Smekal,² G Stefani¹

¹Dipartimento di Fisica and CNISM, Università Roma Tre, Roma, Italy; ²Institut für Angewandte Physik, Vienna University of Technology, Vienna, Austria; ³ETSF and CNISM Milano Bicocca, Milano, Italy; ⁴INFN-CNR and CNISM Università Roma Tre, Roma, Italy

In this work we present the first direct evidence of the plasmon decay via an emission of an electron in the secondary energy region [1]. We have performed (e,2e) and (γ,2e) experiments on Al(100) surface. The secondary electron energy region has been measured in coincidence with the surface and volume plasmon loss peak in the EELS spectrum and with the plasmon satellites in Al 2p photoemission spectrum. In this way it was possible to single out the contribution of surface and bulk plasmon decay to the secondary electron energy region. The coincidence measurements reveal the emission onset at an energy corresponding to the Al Fermi level and a pronounced peak corresponding to the emission from the Al surface state. This result indicates that bulk (or surface) plasmon decays transferring completely its energy and momentum to a single electron in analogy to the photoemission process. In order to investigate the origin of the measured spectral density we have compared experimental data with the calculated Al density of state.

[1] W. Werner, A. Ruocco *et al.* Phys. Rev. B **78** (2008) 233403

5P045

Core-level photoabsorption, photoionization and gas emission in sulfur-containing biomolecules subjected to ionizing radiation

G Simões,¹ FN Rodrigues,^{1,2} LB da Silva,¹ GGB de Souza¹

¹Instituto de Química/UFRJ, Rio de Janeiro, Brazil; ²Instituto Federal do Rio de Janeiro/IFRJ, Rio de Janeiro, Brazil

Amino acids, peptides and proteins are highly susceptible to soft X-ray and electron beam irradiation, undergoing deep chemical transformations under prolonged or intense beam exposure. When subjected to ionizing radiation, these compounds may decompose through a number of pathways, including the release of gaseous species. We hereby report on the experimental determination of XPS and S 1s, N 1s and O 1s NEXAFS spectra of sulfur-containing amino acids (methionine and cysteine), a dipeptide (cystine) and a protein (insulin). The XPS data were obtained at 2500 eV incident photon energy. The samples (powders) were deposited on a carbon sticky paper. In order to search for radiation damage effects, NEXAFS and XPS spectra were also obtained for the same samples, following electron beam (1 keV) or synchrotron radiation (zero order) irradiation. All measurements were made at the Brazilian National Synchrotron Radiation Laboratory (LNLS). Significant spectral changes were observed, particularly in the S 1s and N 1s NEXAFS spectra. During sample irradiation, several gaseous species (H₂, CO₂, CO, H₂S and others) were identified using a quadrupole mass spectrometer.

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5P046

Nondipole photoemission from chiral enantiomers of camphorKP Bowen,¹ WC Stolte,^{1,2} JA Young,³ IN Demchenko,^{1,4} R Guillemin,⁵ O Hemmers,⁶ MN Piancastelli,⁷ DW Lindle¹¹Department of Chemistry, U. of Nevada, Las Vegas, Las Vegas, NV, United States; ²Advanced Light Source, Lawrence Berkeley National Lab, Berkeley, CA, United States;³Jet Propulsion Lab, California Institute of Technology, Pasadena, CA, United States; ⁴Institute of Physics PAS, Warsaw, Poland; ⁵CNRS, Laboratoire de Chimie Physique-Matière et Rayonnement, UMR 7614, Paris, France; ⁶Harry Reid Center for Environmental Studies, University of Nevada, Las Vegas, Las Vegas, NV, United States;⁷Department of Physics and Astronomy, Uppsala U., Uppsala, Sweden

K-shell photoemission from the carbonyl carbon in the chiral molecule camphor has been studied in the region just above the core-shell ionization threshold. Differences between angular distributions of emitted photoelectrons from the two enantiomers are attributed to the influence of chirality combined with nondipole effects in the photoemission process, despite the fact the measurements were taken using *linearly polarized X-rays*. The results suggest the possibility of a new form of linear dichroism. *This work is supported by NSF Award No. PHY-0555699.*

5P047

Direct observation of fullerene plasmon oscillations in momentum spaceS Korica,¹ A Reinköster,¹ M Braune,¹ B Langer,² U Becker¹¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; ²Freie Universität Berlin, Physikalisches und Theoretische Chemie, Berlin, Germany

An extended spherical object which gives rise to standing wave oscillations in the emission intensity of its photoelectrons is exemplified by C₆₀. We performed near-threshold photoionization measurements by photoelectron spectroscopy on C₆₀ in order to demonstrate its HOMO and HOMO-1 threshold behavior. The result was a surprise. The extension of the high-energy sinusoidal behavior toward lower energies revealed a phase jump of $\pi/2$ in the plasmon excitation region. By subtracting the extended undisturbed Cohen-Fano oscillation (an interference effect arising in homonuclear diatomic or spherically symmetric molecules) from the experimental data, we could recover the specific oscillatory behavior of the plasmon excitations directly in momentum space for the first time. In addition, after subtraction of the plasmon oscillations, the shell thickness-dependent beating behavior of the partial cross sections was exhibited much more clearly than demonstrated before. This shows that the Cohen-Fano formula [Phys. Rev. 150, 30 (1966)] provides a very good measure for determining the large-scale coherent photoionization behavior, a prerequisite for the derivation of the energetically more restricted kinds of behavior such as the plasmon oscillations being exhibited in momentum space.

5P048

Target preparation for diffractive X-ray imaging of gas-phase moleculesF Filsinger,¹ L Holmegaard,² J Maurer,² J Thøgersen,² H Stapelfeldt,² HN Chapman,^{3,4} GJM Meijer,¹ J Küpper¹¹Fritz Haber Institute of the Max Planck Society, Berlin, Germany; ²Department of Chemistry, Aarhus University, Aarhus, Denmark; ³Center for Free-Electron Laser Science DESY, Hamburg, Germany; ⁴University of Hamburg, Hamburg, Germany

In 2009 the Linac Coherent Light Source (LCLS) became operational. One envisioned application with this novel hard X-ray free-electron laser is the diffractive imaging of isolated, non-crystallizable bio-molecules in the gas phase. Because a single X-ray laser pulse will completely destroy the molecule, its diffraction pattern needs to be recorded in a single shot. The (electronic) structure of the molecule must not significantly change on the timescale of the laser pulse (< 100 fs) in order to obtain unperturbed diffraction patterns. In order to benchmark radiation damage and the structure retrieval algorithms, we will perform first studies on ensembles of small molecules (e.g. diiodobenzene) at LCLS in spring 2010. In order to observe the diffraction pattern, samples of identical (i.e. oriented) molecules must be prepared. Furthermore, if the target molecules occur as different structural isomers, the individual isomers need to be spatially separated. We have demonstrated the spatial separation of individual structural isomers [1,2] and very strong laser-alignment and mixed field orientation of such molecules [3]. Here, we will discuss how such targets can be prepared, using quantum-state-selection techniques, and applied for X-ray diffraction experiments.

[1] F. Filsinger et al., Phys. Rev. Lett. 100, (2008), 133003

[2] F. Filsinger et al., Angew. Chem. Int. Ed. 48, (2009), 6900

[3] L. Holmegaard et al., Phys. Rev. Lett. 102, (2009), 023001

5P049

XUV pump-probe visualizing ultrafast isomerization of acetylene-vinylidene cations at FLASH

YH Jiang,¹ A Rudenko,² L Foucar,² M Kurka,¹ KU Kühnel,¹ O Herrwerth,³ M Lezius,³ M Kling,³ JVJ van,⁴ A Belkacem,⁴ K Ueda,⁵ S Düsterer,⁶ R Treusch,⁶ CD Schröter,¹ R Moshhammer,¹ J Ullrich¹

¹Max-Planck-Institut für Kernphysik, Heidelberg, Germany; ²Max-Planck Advanced Study Group at CFEL, Hamburg, Germany; ³Max-Planck-Institut für Quantenoptik, Garching, Germany; ⁴Lawrence Berkeley National Laboratory, Berkeley, United States; ⁵Institute of Multidisciplinary Research for Advanced Materials, Seidai, Japan; ⁶DESY, Hamburg, Germany

Isomerisation is an elementary chemical reaction where the conformation of a molecule evolves continuously through a sequence of transient species that are neither reactants nor products, but finally turning the former into the latter. Using a XUV pump-probe setup in combination with a reaction microscope we were able to visualize the isomerisation of acetylene cations ($\text{HC}=\text{CH}^+$) that were created by ionization of neutral molecules in the gas phase during the pump pulse (38 eV photon energy). This has been achieved by analyzing the C^++CH_2^+ fragmentation channel, which serves as an indicator for the transfer of a proton from one end of the molecule to the other end, as function of the pump-probe delay time. We obtained a mean isomerization time of about 50 fs.

5P050

iPEPICO studies on atmospherically relevant $\text{S}_x\text{O}_y\text{Cl}_z$ ions

S Borkar,¹ L Ooka,¹ A Bodi,² T Gerber,² B Sztáray¹

¹Department of Chemistry, University of the Pacific, Stockton, CA, United States; ²Paul Scherrer Institut, PSI Villigen, Switzerland

Atmospheric sulfur chemistry has immense significance to the biosphere. In order to model interactions between the sulfur and halogen cycles in atmospheric models, reliable thermochemical data is needed for the various $\text{S}_x\text{O}_y\text{Cl}_z$ neutrals and ions. TPEPICO and iPEPICO experiments were performed on SCl_2 , S_2Cl_2 , SOCl_2 , and SO_2Cl_2 to derive heats of formation of the various $\text{S}_x\text{O}_y\text{Cl}_z^+$ fragment ions and their neutral counterparts to fill this gap. The iPEPICO experiments were performed on the newly built VUV beamline of the Swiss Light Source. In dissociative photoionization, SCl_2 leads to SCl^+ , the heat of formation of which is determined. In the iPEPICO experiment, S_2Cl_2 leads to S_2Cl^+ and then to S_2^+ in consecutive dissociation steps. In this case both the end product and the neutral precursor has reliable literature h.o.f., they are used to characterize the product energy distribution, and the data were found to agree with 3-D translation. For SOCl_2 , the picture is similar, except that the thermochemistry of SO^+ is much better known and is not consistent with the h.o.f. of neutral SOCl_2 for which a more reliable number is given. The heat of formation of SO_2Cl^+ is derived from the SO_2Cl_2 neutral heat of formation. From our results, not only the sulfur-chlorine ionic bond energies are measured, but since the four systems are interconnected through a loss of oxygen, S=O bond energies are also determined indirectly.

5P051

Ab initio determination of $K\alpha$ line strengths, energies and spectator intensities in transition metal atoms

JA Lowe,¹ CT Chantler¹

¹School of Physics, University of Melbourne, Parkville, Victoria, Australia

Photoionisation of a K shell electron leads to a characteristic photoemission spectrum. Following core ionisation, the abrupt change in potential can lead to secondary ionisation of an outer shell electron in a phenomenon known as shake off. The resultant spectator vacancies give rise to the asymmetric $K\alpha$ profile and satellite lines. Despite wide application of $K\alpha$ radiation and extensive theoretical efforts, discrepancies remain between *ab initio* atomic structure calculations and experiment, especially in complex atoms. Multiconfiguration-Dirac-Fock (MCDF) calculations have proven highly accurate in determination of energies and transition strengths. Performing the equivalent calculations on more complex atoms has, until recently, yielded poor agreement with experiment. New implementations of theoretical advances have allowed determination of line positions to accuracies of <0.1eV in copper, compared with 1-2eV previously. Using the MCDF method we provide a detailed analysis of the copper and titanium $K\alpha$ spectra, including calculations for multiple states with spectator vacancies. New methods have been developed for handling highly excited atoms with 3 or more open shells. The higher degree of convergence obtainable has also allowed new *ab initio* calculations of spectator intensities in far better agreement with experiment.

[1] Chantler, Hayward, Grant, Phys. Rev. Lett. 103 [2009] 123002

[2] J. A. Lowe, C. T. Chantler, I. P. Grant, 'Theoretical determination of characteristic X-ray lines and the titanium K α spectrum', submitted [PRL]

5P052

A VUV photoionization organic aerosol mass spectrometric study with synchrotron radiation

W Fang,¹ L Gong,¹ J Chen,¹ G Chu,¹ L Cao,¹ X Shan,¹ F Liu,¹ Z Wang,² L Sheng¹

¹National Synchrotron Radiation Laboratory, School of Nuclear Science and Technology, University of Science and Technology of China, Hefei, Anhui, China; ²Laboratory of Environmental Spectroscopy, Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui, China

A photoionization aerosol time-of-flight mass spectrometer (ATOFMS) has been developed for real-time analysis of organic compounds in aerosol particles using tunable vacuum ultraviolet (VUV) synchrotron radiation. Aerosol particles can be sampled directly from atmospheric pressure and are focused through an aerodynamic lens assembly into the mass spectrometer. The particles are vaporized when they impact on a heater, and then the nascent vapor is softly photoionized by synchrotron radiation. The degree of fragmentation of molecule can be controlled either by the heater temperature or by the energy of the ionizing photon. Thus, fragment-free tunable VUV mass spectra are obtained by tuning the photon energy close to the ionization energies (IEs) of sample molecules. The direct determination of the IEs of benzophenone (9.07 eV), salicylic acid (8.72 eV), and urea (9.85 eV) are measured from the photoionization efficiency spectra with uncertainties of ± 50 meV. Ab initio calculation has been employed to predict the theoretical ionization energy.

5P053

Photoemission from valence bands of transition metal-phthalocyanine

MH Shang,¹ M Nagaosa,¹ SI Nagamatsu,² S Kera,¹ T Fujikawa,¹ N Ueno¹

¹Graduate School of Advanced Integration Science, Chiba University, Yayoi-cho, Inage, Chiba, Japan;

²The University of Electro-Communications, Chofugaoka, Chofu-shi, Tokyo, Japan

Transition metal-phthalocyanines (TMPcs) are promising materials for photovoltaic devices, organic semiconductors, optoelectronic/magnetic materials and so forth. However, so far, systematic information on the electronic structure of TMPcs is so limited. The impact of photoelectron angular distribution (PAD) of ultraviolet photoelectron spectrum (UPS) have been studied by using multiple-scattering theory on centered TMs. The calculated PAD from the highest occupied molecular orbital (HOMO) which has no contribution from transition metal is compared for various gaseous TMPcs. Our calculated results show reasonable agreement with the observed spectra. The calculated result for NiPc shows a quite different angular pattern from other TMPc. This theoretical interesting behavior can be explained by the framework of the final state effects, where excited photoelectrons can be differently scattered from the central TM's.

5P054

Valence photoionization of LiCl monomer and dimer

J Niskanen,^{1,2} S Urpelainen,^{1,3} S Aksela,¹ H Aksela,¹ O Vahtras,² V Carravetta,⁴ H Ågren²

¹Department of Physics, University of Oulu, Oulu, Finland; ²Department of Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden; ³MAX-lab, Lund University, Lund, Sweden; ⁴CNR - Institute of Chemical Physical Processes, Pisa, Italy

In this work [1] we studied the behavior of valence photoionization cross sections of LiCl monomer and dimer. By introducing Kr to the interaction region for calibration, the relative partial photoionization cross sections for molecular valence orbitals could be measured as a function of photon energy between 15 and 35 eV. A theoretical method based on projection of the excited states on a set of square-integrable basis functions [2,3] was used to compute the ionization partial cross sections in independent particle independent channel approximation. The experiments were carried out on the FINEST gas phase branch line on the I3 beamline of the 700 MeV MAX-III electron storage ring. The trend of the cross section for monomer lines and dimer were reproduced well by the calculations, but a shift of 6.5 eV was seen between the calculated and experimental maxima of the ionization cross sections.

[1] J. Niskanen, S. Urpelainen, S. Aksela, H. Aksela, O. Vahtras, V. Carravetta and H. Ågren, Phys. Rev. A **81**, 043401 (2010).

[2] I. Cacelli, V. Carravetta, A. Rizzo, and R. Moccia, Phys. Rep. **205**, 283 (1991) and references therein.

5P055

Photoelectron angular distribution and linear magnetic dichroism in the 4p photoemission from Rb atoms

J Niskanen,^{1,2} S Urpelainen,¹ K Jänkälä,¹ J Schulz,^{1,3} S Heinäsmäki,¹ S Fritzsche,^{1,4} NM Kabachnik,^{1,5} S Aksela,¹ H Aksela¹

¹Department of Physics, University of Oulu, Oulu, Finland; ²Department of Theoretical Chemistry, Royal Institute of Technology, Stockholm, Sweden; ³Center for Free-Electron Laser Science (CFEL) at DESY, Hamburg, Germany; ⁴GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany; ⁵Institute of Nuclear Physics, Moscow State University, Moscow, Russia

In this work [1] the angular distribution of photoelectrons and linear magnetic dichroism in the angular distribution (LMDAD) for the 4p photoemission from Rb atoms in the ground state, oriented by laser pumping, were measured at selected photon energies in the photon energy range from 50 to 100 eV. The experimental results were compared with the multiconfiguration Dirac-Fock (MCDFF) calculations. In general, the calculations reproduced well the experimental values of the angular anisotropy parameters of 4p photoelectrons and the relative LMDAD as well as their energy dependence in the considered energy range, except a shift of 10 eV. In the energy dependence of LMDAD, we observed the zero-crossing connected with the Cooper minimum of the cross section. In the study we showed that the zero-crossing of the LMDAD as a function of energy is connected with the Cooper minimum in the cross section. This fact can be used for an accurate determination of the position of the Cooper minimum. [1] J. Niskanen, S. Urpelainen, K. Jänkälä, J. Schulz, S. Heinäsmäki, S. Fritzsche, N. M. Kabachnik, S. Aksela and H. Aksela Phys. Rev. A **81**, 013406 (2010).

5P056

Atomic data for VUV lines of astrophysical interest in singly ionized rhodium

P Quinet,^{1,2} E Biémont,^{1,2} P Palmeri,¹ L Engström,³ H Hartman,⁴ H Lundberg,³ H Nilsson⁴

¹Astrophysique et Spectroscopie, Université de Mons - UMONS, Mons, Belgium; ²IPNAS, Université de Liège, Liège, Belgium; ³Department of Physics, Lund Institute of Technology, Lund, Sweden; ⁴Lund Observatory, Lund University, Lund, Sweden

The investigation of high resolution astronomical spectra depends directly on reliable atomic data such as transition probabilities and oscillator strengths. Although many are now available from modern experimental techniques or sophisticated theoretical methods, they are still insufficient to meet all the needs of astrophysicists. This is particularly true for singly ionized rhodium for which no radiative data have been published so far in the literature despite the fact that several Rh II lines were identified in different astrophysical spectra. In the present contribution, we report on calculations of radiative decay rates for Rh II lines appearing in the VUV region between 100 and 200 nm using a relativistic Hartree-Fock approach in which we have included the most important relativistic and core-polarization effects. The reliability of the theoretical model used for the computations has been tested by comparison with 17 experimental radiative lifetimes measured with the time-resolved laser-induced fluorescence technique at the Lund Laser Centre in Sweden.

5P057

Manifestation of PCI in cascade double Auger decay of Ar 2p holes

S Sheinerman,¹ P Lablanquie,² F Penet,² Y Hikosaka,³ T Kaneyasu,⁴ E Shigemasa,⁴ K Ito,⁵ J Palaudoux²

¹Maritime Technical University, St Petersburg, Russian Federation; ²LCPMR, Université Pierre & Marie Curie, Paris, France; ³Niigata University, Niigata, Japan; ⁴UVSOR, IMS, Okazaki, Japan; ⁵PF, IMSS, Tsukuba, Japan

The photoionization of an Ar 2p inner shell followed by cascade Auger decay with emission of two electrons is investigated both experimentally and theoretically. Such a process leads to triply charged final ionic states with three electrons in the continuum. Electron spectra of the emitted electrons are known to be influenced by post collision interaction (PCI) which results from the interaction between all charged particles: photo and Auger electrons and ionic field which varies during the Auger decay. Our previous investigations of PCI in double Auger decay examined the case of direct double Auger (DDA) emission when the two Auger electrons are emitted simultaneously. The present study faces the case of cascade double Auger (CDA) decay when the emission of the electrons occurs subsequently through creation and decay of intermediate quasi-stationary states. On the experimental side, we detect in coincidence the three electrons released in the process with a magnetic bottle time-of-flight spectrometer. Theoretically, we carried out the calculation of the electron spectra based on a quantum mechanical eikonal model of PCI in the CDA processes. Results of both measurement and calculation show that the PCI distortion of the electron spectra depends strongly on the widths of the inner shell 2p vacancy Γ_1 and of the intermediate state Γ_2 as well as on the kinematics of process, i.e. the velocities of the three emitted electrons. A complete analysis of the results will be presented at the conference.

5P058

Vibrational and rotational excitations associated with inner-shell ionization in small molecules

ES Borisenko,¹ XO Brykalova,¹ YS Krivosenko,¹ RB Lazurkov,¹ DA Mistrov,¹ AA Pavlychev¹¹Department of Physics, St. Petersburg State University, St. Petersburg, Russian Federation

Spectral distributions of vibrational excitations associated with inner-shell ionization in CO, N₂, CO₂, and SF₆ are investigated and reported. Special emphasis is put on the non-Franck-Condon effects originated from (1) interference of the primary and scattered photoelectron waves in respect to symmetry of molecular vibrations and (2) coupling of valence-excited-core-ionized states via autoionization to the core-hole ionization continuum. Using the VDFN method the distributions are computed and compared with the experimental data. It is shown that population of vibrational states (1) varies strongly at the shape resonance, (2) oscillates around the sudden limits far from the threshold, and (3) demonstrates "anti-FC" behavior for high v'-states due to the relaxation of valence shells. The work of the relaxation mechanism is described. In particular, the population of v'=7 in CO is enhanced nearly 10³ times relative to the FC value. Dependence of the non-FC deviations on symmetry of molecular frame motions is found to be important. The essential effect of zero-point molecular motion on photoelectron-recoil-induced molecular rotations is predicted. Perspectives in high-energy photoelectron spectroscopy of free molecules and more precise determination of the spectroscopic parameters of their core-ionized states are discussed.

5P059

Efficiency of the extraction algorithm in grating-based X-ray phase imaging

Z Wang,¹ P Zhu,¹ X Liu,¹ K Zhang,¹ Y Hong,¹ Q Yuan,¹ W Huang,¹ Z Wu²¹Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China; ²National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui, China

We present here the concept of the shifting curve in the grating-based phase contrast imaging [1]. A novel phase extraction algorithm, named "Reverse-Projection" (RP) technique, has been proposed, based on the linear approximation of the shifting curve. The RP technique has been validated by experimental results, in agreement with those obtained by the phase-stepping (PS) technique [2]. In this contribution, we assess the efficiency of the RP technique, in terms of the minimum detectable refraction angle with a sufficient signal-to-noise ratio as a function of the available photon flux. The photon statistics affects the detected intensities and impose a limit to the refraction angle. We determine the relation between the incident photon number and the detection limit, and define a figure of merit for a monochromatic spherical wave illumination. The dependence of the figure of merit on the optical system parameters is also discussed. Numerical simulations provided also a quantitative insight of the efficiency of the RP technique.

1. Z. Wang, X. Liu, P. Zhu, K. Zhang, W. Huang, Q. Yuan, Y. Hong, X. Ge, Z. Wu (to be submitted to Optics Express).
2. P. Zhu, K. Zhang, Z. Wang, Y. Liu, X. Liu, Z. Wu, S. A. McDonald, F. Marone, M. Stampanoni (submitted to PNAS).

5P060

Spectral distribution of v'₁ - and v'₃ -vibrational excitations associated with C and O K shells photoionization in the CO₂ molecule

ES Borisenko,¹ DA Mistrov,¹ AA Pavlychev¹¹Department of Physics, St. Petersburg State University, St. Petersburg, Russian Federation

The non-Franck-Condon intensity of vibrational transitions in the shape resonance vicinity is a natural consequence of intramolecular interference of the primary and scattered photoelectron waves and zero-point molecular motions. Special emphasis is put on difference in spectral distributions of symmetric and asymmetric stretching excitations. Photoemission from CO₂ is the most favorable probe of the symmetry dependence because v'₁ - and v'₃ -modes dominate in the C and O K shell ionization producing strong non-FC and almost FC distributions (f₁ and f₃) at the 4⁺_u shape resonance. The influence of symmetric stretching on inner-shell ionization is studied in detail. Using the VDFN model [1] the spectral distributions f₁ and f₃ in CO₂ are computed and compared. f₃ demonstrates strong non-FC behavior below and above the 4⁺_u shape resonance and approaches to the FC distribution at the resonance. This anomalous distribution of v'₃ -excitations is assigned with the interplay of threshold and interferential effects on O 1s ionization. The studies of f₁ confirm the results of the work [1]. The regularities in spectral distributions of symmetric and asymmetric stretching vibrations associated with inner-shell ionization in linear triatomics are discussed.

- [1] A. A. Pavlychev, D. A. Mistrov, J. Phys. B, 42 055103 (2009)

5P061

The limits of the muffin-tin approximation for XANES simulations of highly anisotropic systems

W Xu,¹ D Chen,¹ W Chu,¹ Z Wu,^{1,2} A Soldatov,³ A Mottana,^{4,5} MF Brigatti,⁶ A Marcelli⁴

¹BSRF, Institute of High Energy Physics, Beijing, China; ²NSRL, University of Science and Technology of China, Hefei, China; ³Center for nanoscale structure of matter, Southern Federal University, Rostov-na-Donu, Russian Federation; ⁴INFN-LNF, Roma, Italy; ⁵Dipartimento di Scienze Geologiche, Università degli Studi Roma Tre, Roma, Italy; ⁶Dipartimento di Scienze della Terra, Università di Modena e Reggio Emilia, Modena, Italy

The X-ray absorption spectra are usually described in the framework of one-particle approximation with the atomic potential approximated by spherically separated regions, i.e., the classical muffin-tin approximation. The approximation is valid for most cases but its inadequacy has been already pointed out in systems with an open lattice structure in contrast with the closely packed crystalline structures and in systems characterized by a reduced symmetry (e.g. Butler, 1992). Micas are natural and synthetic systems characterized by an open lattice structure with a high cation coordination (>9), large first neighbouring distances around the interlayer ions (>3 Å) and an anisotropic layered structure with quite low crystal symmetry such as C_2 or $C_{2/m}$. Therefore micas represent a perfect and challenging model to test the muffin-tin approximation and the construction of more sophisticated atomic potentials. We will show the failure of the muffin-tin approximation in angular polarized XANES at the *K* edge of potassium and, we will demonstrate that the inadequacy of the muffin-tin potential for calculations of spectra polarized along the *c* axis in layered materials.

5P062

Large-scale relativistic configuration-interaction calculations for the 2s-2p and 3s-3p transition energies of xenon ions

MH Chen,¹ KT Cheng¹

¹Lawrence Livermore National Laboratory, Livermore, CA, United States

The 2s-2p transition energies for Li-, Be- and B-like xenon and 3s-3p transition energies for Na- and Mg-like xenon are calculated using the relativistic configuration-interaction (RCI) method. These calculations are based on the no-pair Hamiltonian that includes both Coulomb and Breit interactions and use one-electron B-spline orbitals as basis functions. Large-scale RCI expansions include single and double excitations from the valence and core electrons and reach 350,000 configurations for accurate evaluations of relativistic correlation energies. Along with quantum electrodynamic (QED) and mass polarization (MP) corrections calculated here, our transition energy results are in very good agreement with those from high precision EBIT measurements.

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5P063

Core-electron tunneling in diatomics interacting with intense ultrashort-pulsed XUV and X-ray radiation: theoretical studies

O Ponomarenko^{1,2}

¹ARC CoE CXS, The School of Physics, The University of Melbourne, Melbourne, Victoria, Australia; ²ARC CoE CXS, The School of Physics, The Monash University, Melbourne, Victoria, Australia

New sources of intense XUV/X-ray ultra-short pulse radiation - X-ray free-electron and HHG lasers - present a unique opportunity to develop time-resolved structure determination schemes. These techniques would make it possible to trace the time evolution of the electronic density in molecular systems, and identify signatures of core-electron transitions during the probe pulse. The field of XFEL is sufficient to influence the migration by field-induced bound-state tunnelling of core hole states generated by one-photon photoionization. Since molecular imaging experiments at atomic resolution are sensitive to the core-electron density in the target, any modification of this density has potential implications for the imaging experiments using femtosecond X-ray pulses. In this presentation, we provide an illustration of the effects of field-induced core-hole transport on X-ray scattering properties in molecular systems. As an example, we consider inter-well tunneling of a core electronic density through the Coulomb barrier between nuclei in a single-electron dicarbon molecular ion driven by intense extreme-ultraviolet laser field. We employ a simple numerical two-state model which is further elaborated and supported by a three-dimensional model based on numerical solution of the time-dependent Schrödinger equation. The laser field parameters determining core-hole tunneling rates are found to be scalable for the higher intensity/shorter wavelength regimes. The implications of this study on the reconstruction of molecular structures by analysis of scattering data in single-shot X-ray free-electron laser experiments are discussed.

5P064

Theoretical analysis of spin-orbit and exchange interactions in S and P 2p excitations of CS, SO₂ and PF₃

M Tashiro,¹ M Ehara,¹ N Kosugi¹¹Institute for Molecular Science, Okazaki, Japan

Interpretation of experimental 2p inner-shell excitation spectra is often complicated because of the molecular-field (MF) and spin-orbit (SO) splittings and the core-valence exchange (EX) or singlet-triplet splitting; especially in the second-row elements, the SO and EX splittings are comparable around 1-2 eV [Kosugi, JES **137-140**(2004)335]. When the SO splitting is larger than the EX splitting, the 2p_{3/2} and 2p_{1/2} bands show its intensity ratio of 2:1 as expected from the jj coupling scheme. On the other hand, when the EX splitting is much larger than the SO splitting, only one absorption peak corresponding to the singlet-dominant state is observable. In this work, we investigate absorption spectra for S 2p excitations in CS and SO₂, and P 2p excitations in PF₃. The CASSCF method combined with the state-interacting method for spin-orbit effect was employed. In the S 2p excitations of CS and SO₂, for the perpendicular transition, the lower energy band (2p_{3/2}) is stronger than the higher energy band (2p_{1/2}). For the parallel transition, however, the higher band is stronger than the lower band, indicating that the larger 2p-π* exchange interaction violates the jj coupling scheme. Furthermore, in the P 2p excitation in PF₃, we have successfully confirmed a complete breakdown of the jj coupling scheme as predicted experimentally [Kosugi et al, CPL **265**(1997)490].

We would like to acknowledge encouragements of our calculations on SO₂ by Takaki Hatsui, CS by Stefano Stranges and Robert Richter, and PF₃ by Yongfeng Hu and Ralph Puettner.

5P065

Theoretical calculation of molecular photoionization – application of the ab initio R-matrix method

M Tashiro¹¹Institute for Molecular Science, Okazaki, Japan

The R-matrix method [1] has been widely used for theoretical calculation of electron-atom, and electron-molecule collisions. Though the R-matrix method was also formulated to treat photoionization problem [2], it has been mainly applied to photoionization of atoms, but not molecule. We have implemented a program [3] for calculation of molecular photoionization properties, e.g., cross section and anisotropy parameter, based on the UK R-matrix codes [4] which has been developed by Tennyson et al for electron-molecule collision problem. As described in ref.[2], final state wavefunction of photoionization process is obtained based on electron molecular-ion scattering calculation, where the wavefunctions of molecular-ion are expressed in CI expansion. We will show the benchmark results for valence and inner-shell photoionization cross sections for N₂ and NO as well as other small molecules.

[1] Burke, Hibbert and Robb, J. Phys. B: At. Mol. Phys. **4**, 153 [1971].

[2] Burke and Taylor, J. Phys. B: At. Mol. Phys. **8**, 2620 [1975].

[3] Tashiro, J. Chem. Phys. **132**, 134306 [2010].

[4] Morgan, Tennyson, and Gillan, Comput. Phys. Commun. **114**, 120 [1998].

5P066

Influence of geometric aberrations on XUV attosecond pulses

C Bourassin-Bouchet,¹ S de Rossi,¹ F Delmotte,¹ P Chavel¹¹Laboratoire Charles Fabry, Institut d'Optique, Univ Paris sud, CNRS, RD128 Campus Polytechnique, Palaiseau, France

Attosecond light pulses (1 as = 10⁻¹⁸ s) can nowadays be produced by high-harmonic generation in the extreme ultraviolet. Focusing such attosecond pulses is essential for numerous applications, including attosecond pulse duration measurements. Generally toroidal grazing incidence mirrors and near normal incidence multilayer mirrors are used to refocus these pulses. But as any optical component, these mirrors can introduce geometric aberrations, so that the wavefront of a refocused ultra-short pulse is not spherical anymore. Such effects can be dramatic when considering attosecond pulses. Since a 100 as pulse is 30 nm thick, a variation greater than 30 nm of the optical paths is sufficient to significantly stretch the pulse. Consequently even weak aberrations can lead to strong spatio-temporal distortions of the attosecond pulses, which results in a loss of the attosecond structure. We performed a numerical study of such effects induced by current mirrors [1].

[1] C. Bourassin-Bouchet et al, «Spatio-temporal distortions of attosecond pulses», J. Opt. Soc. Am. A (to be published).

5P068

Core-electron excitation and fragmentation processes of acetic-acid clusters in the oxygen K-edge region

K Tabayashi,¹ K Yamamoto,¹ T Maruyama,¹ H Yoshida,¹ K Okada,¹ Y Tamenori,² IH Suzuki,³ T Gejo,⁴ K Honma⁴

¹Hiroshima University, Higashi-Hiroshima, Japan; ²JASRI/Spring-8, Hyogo, Japan; ³National Metrology Institute of Japan/AIST, Tsukuba, Japan; ⁴University of Hyogo, Hyogo, Japan

In order to examine inner-shell electron excitation and induced chemical processes of strongly hydrogen-bonded (HB) molecular clusters, time-of-flight (TOF) fragment-mass and excitation spectra of deuterium-labeled acetic-acid-d (AAD) have been studied under the effusive and cluster beam conditions. With $O1s_{CO}^{-1}\pi_{CO}^*$ excitation at 532 eV, sample TOF spectra of AAD clusters were compared with those of free molecules. Intensity enhancement of the CH_3^+/CH_3CO^+ fragments and growth of the mixed-cluster cations, $M_nD^+/M_nCH_3CO^+$ could be ascertained in the cluster beams, where AAD molecule is denoted by M. Cluster-specific excitation spectra have been generated by monitoring partial-ion-yields of the mixed-cluster cations. Resonance transitions of $O1s_{CO/OH}^{-1}\pi_{CO}^*$ were found to shift in energy upon clusterization. The production of M_nD^+ can be attributed to a low energy pathway of deuteron (proton) transfer within the clusters made up of a stable dimer-unit with doubly-bridged HBs. The CH_3^+/CH_3CO^+ production clearly shows that a local-fragmentation mechanism as previously proposed is also realized in the present small AAD clusters.

5P070

Interatomic Coulombic decay of Ne-Ar dimers following Auger decay

T Ouchi,¹ K Sakai,¹ I Higuchi,² H Fukuzawa,¹ X Liu,¹ M Okunishi,¹ K Ueda,¹ H Iwayama,³ K Nagaya,³ M Yao,³ D Zhang,⁴ D Ding,⁴ M Schöffler,⁵ T Mazza,^{1,6} Y Tamenori,² N Saito⁷

¹IMRAM, Tohoku Univ., Sendai, Japan; ²JASRI, Sayo, Japan; ³Dept. of Phys., Kyoto Univ., Kyoto, Japan; ⁴Jilin Univ., Changchun, China; ⁵LBNL, Berkeley, United States; ⁶Univ. of Milan, Milan, Italy; ⁷NMIJ, AIST, Tsukuba, Japan

Core-level photoionization of clusters leads to Auger decay and then may cause interatomic Coulombic decay (ICD) [1]. In this study, we have investigated these electronic relaxation processes for Ne-Ar dimers. We used the linearly polarized soft X-ray from beam line 27SU at SPring-8. Ne-Ar dimers were produced by expanding Ne and Ar mixed gases. We used electron-ion coincidence technique to get the three-dimensional momenta of ions and electrons. We observed ICD processes following $Ar L_{2,3}M_1M_1$ Auger decay; $Ar^{2+}(3s^2) - Ne \rightarrow Ar^{2+}(3p^2\ ^1D) - Ne^+(2p^1)$ and $Ar^{2+}(3s^2) - Ne \rightarrow Ar^{2+}(3p^2\ ^3P) - Ne^+(2p^1)$. Our results are the first observation of the ICD processes in which three electrons are participated.

[1] R. Santra and L. S. Cederbaum, *Phys. Rev. Lett.* **90**, 153401 (2003)

5P071

Photoelectron and ICD electron emissions after KLL Auger decay in neon clusters

K Sakai,¹ H Fukuzawa,¹ XJ Liu,¹ M Okunishi,¹ K Ueda,¹ H Iwayama,² K Nagaya,² M Yao,² IH Suzuki,³ Y Morishita,³ N Saito,³ I Higuchi,⁴ Y Tamenori⁴

¹IMRAM, Tohoku University, Sendai, Japan; ²Dept. of Phys., Kyoto University, Kyoto, Japan; ³NMIJ, AIST, Tsukuba, Japan; ⁴JASRI, Sayo, Japan

Ne 1s photoionization of Ne clusters leads to Auger decay and then may cause interatomic Coulombic decay (ICD) [1]. We have investigated these sequential processes using three-dimensional momentum resolved electron-ion coincidence. The experiment was carried out on the c branch of the soft X-ray photochemistry beam line 27SU at SPring-8. The cluster beam included the clusters with the average cluster size $\langle n \rangle \sim 3$ and 24. Electron-ion multi-coincidence signals were recorded with linearly polarized light at photon energy of 890 eV, i.e., ~ 20 eV above the Ne 1s ionization threshold. Measured photoelectron angular distributions depend on the direction of the polarization vector \mathcal{E} , but do not depend on the direction of ion ejection. The value of the anisotropy parameter is smaller with increasing cluster size. The deviation from the value of 2 which is expected for atomic Ne 1s photoionization may be attributed to multiple scattering effects in clusters. ICD electron angular distributions depend on neither the direction of ion ejection nor the direction of the polarization vector \mathcal{E} , indicating that there is no selectivity in orientation of emitting the ICD electron.

The present experiment has been carried out with the approval of JASRI and partially supported by JSPS.

[1] R. Santra and L. S. Cederbaum, *Phys. Rev. Lett.* **90**, 153401 (2003).

5P073

The observation of electronic energy bands in argon clusters

M Förstel,^{1,2} M Mucke,¹ T Arion,¹ T Lischke,¹ S Barth,¹ V Ulrich,¹ G Öhrwall,³ O Björneholm,³ U Hergenhahn,¹ AM Bradshaw^{1,4}

¹Max-Planck-Institut für Plasmaphysik, EURATOM Association, Garching, Germany; ²Max-Planck-Institut für Kernphysik, Heidelberg, Germany; ³Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden; ⁴Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The electronic structure of ordered bulk matter is characterized by the formation of electronic bands, the energy of which depends on the crystal momentum k . Determining the dispersion, i.e. the change of energy with respect to k of the initial state, is an important field in solid state physics. In this study we have used clusters to investigate, how large a piece of matter needs to be in order to show a dispersion resulting from electronic bands. The 3p valence region of argon clusters has been investigated with photoemission near the photoionization threshold. A strong feature between 14.6 and 15.3 eV binding energy shows a photon energy dependence indicative of electronic energy band dispersion. A similar feature at approximately the same binding energy and with a similar dispersion occurs in photoemission spectra of both the ordered and disordered solids. The effect is already fully developed for mean cluster sizes of about 150 - 200 atoms, thus showing an early onset of bulk-like electronic properties.

5P074

Temperature-dependent structuring of Au-Pt bimetallic nanoclusters on a thin film of $\text{Al}_2\text{O}_3/\text{NiAl}(100)$

MF Luo,¹ CC Wang,¹ CY Ho,¹ CT Wang,¹ WR Lin,¹ GR Hu,¹ YJ Hsu²

¹Department of Physics, National Central University, Jhongli City, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu City, Taiwan

Au-Pt bimetallic nanoclusters on a thin-film $\text{Al}_2\text{O}_3/\text{NiAl}(100)$ undergo significant structural evolution on variation of temperature. Au and Pt deposited from the vapor onto thin-film $\text{Al}_2\text{O}_3/\text{NiAl}(100)$ at 300 K preferentially form bimetallic nanoclusters (diameter ≤ 6.0 nm and height ≤ 0.8 nm) with both Au and Pt atoms on the cluster surface; the evidence from photoelectron spectra shows atypically small binding energy and line width of Au 4f core levels. These bimetallic clusters are structurally ordered, have a fcc phase and grow with their facets either {111} or {001} parallel to the $\text{Al}_2\text{O}_3(100)$ surface. Upon annealing the clusters to 400–500 K, both the binding energy and line width of Au 4f increases, indicating migration of the Au atoms toward the cluster surface and thus formation of a Pt core–Au shell structure. Annealing the sample to 500–650 K reorients the bimetallic clusters all clusters have their {001} facets parallel to the oxide surface — and induces oxidation of Pt.

5P075

XAS studies of active sites on nanosize TiO_2 for photocatalytic degradation of CHCl_3

TL Hsiung,¹ HP Wang,^{1,2} YL Wei³

¹Department of Environmental Engineering, National Cheng Kung University, Tainan, Taiwan; ²Sustainable Environment Research Center, National Cheng Kung University, Tainan, Taiwan; ³Department of Environmental Science and Engineering, Tunghai University, Taichung, Taiwan

To decrease the risk of water-borne diseases, chlorine is often used as a disinfectant in a potable water supply system. Since 1976, the disinfection byproducts (DBPs) such as trihalomethanes (THMs) (the large quantity of DBPs) have been found in drinking water treatment processes. Note that chloroform (one of THMs) is carcinogen in rodents as proposed by the U.S. National Cancer Institute. In the separate experiments, we have found that the THMs can be photocatalytically degraded on nanosize TiO_2 . However, nature of the photoactive sites is still not well understood. A molecule-scale understanding of photocatalytic active sites on TiO_2 nanoparticles was, therefore, studied by X-ray absorption near edge structure spectroscopy. The component fitted pre-edge spectra show that A_1 (4969 eV), A_2 (4971 eV) and A_3 (4972 eV) can be distinguished as four-, five-, and six- coordinated Ti species on the nano- and subnano-size (cluster and atomic dispersed) TiO_2 , respectively. Notably, the A_2 sites which are the main photocatalytic species on the nanosize TiO_2 account for >90% of the total reactivity [$7.2 \text{ ppmCHCl}_3/\text{gTiO}_2 \cdot \text{hr}$] for photocatalytic degradation of trace CHCl_3 in drinking water.

5P076

Anisotropy of photoelectron emission from giant xenon cluster irradiated by EUV free-electron laser at SPring-8

K Nagaya,^{1,2} A Sugishima,^{1,2} Y Mizoguchi,^{1,2} H Iwayama,^{1,2} M Yao,^{1,2} H Fukuzawa,^{2,3} K Motomura,^{2,3} A Yamada,^{2,3} K Ueda,^{2,3} N Saito,^{2,4} P Piseri,^{2,3,5,6} T Mazza,^{2,3,5,6} M Devetta,^{2,3,5,6} M Coreno,^{2,7} M Nagasono,² K Tono,² M Yabashi,² T Ishikawa,² H Ohashi,^{2,8} H Kimura,^{2,8} T Togashi,^{2,8} Y Senba⁸

¹Dept. of Phys., Kyoto University, Kyoto, Japan; ²RIKEN XFEL, Sayo, Japan; ³IMRAM, Tohoku University, Sendai, Japan; ⁴NMIJ, AIST, Tsukuba, Japan; ⁵Università di Milano, Milano, Italy; ⁶CIMAINA, Milano, Italy; ⁷CNR-IMIP, Roma, Italy; ⁸JASRI, Sayo, Japan

Recent developments of the free electron laser (FEL) light sources based on self-amplified spontaneous-emission (SASE) enable us to study the multiple ionization processes of atoms, molecules and clusters in vacuum ultraviolet (VUV) and extreme ultraviolet (EUV) regions. Now SPring-8 Compact SASE Source (SCSS) test accelerator is in operation and it provides intense EUV-FEL pulses in the wavelength region of 51 - 61 nm. In this study, we investigate the multiple photoionization processes of giant xenon clusters ($\langle N \rangle \sim 10000$) induced by EUV-FEL pulses at $\lambda = 52 \text{ nm}$ ($h\nu = 24 \text{ eV}$) by using a photoelectron spectroscopy. Four time-of-flight type electron spectrometers at two detection angles have been utilized to determine anisotropy of electron emission. We found the anisotropic electron emission from giant xenon cluster in addition to the signature of the frustration of photoionization of clusters.

We are grateful to the SCSS Test Accelerator Operation Group at RIKEN for continuous support in the course of the studies.

5P077

Gas-to-cluster and gas-to-solid shifts in S 2p and F 1s excited SF₆XO Brykalova,¹ R Fleisch,² E Seardarogu,² F Blobner,³ P Feulner,³ AA Pavlychev,¹ E Ruehl²¹Department of Physics, St. Petersburg State University, St. Petersburg, Russian Federation; ²Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Berlin, Germany; ³Physik-Department E20, TU München, Garching, Germany

Special emphasis is put on X-ray absorption near the S 2p and F 1s edges in the SF₆ molecule, where the molecular units are either bound in free variable size van der Waals clusters or in the solid. The experimental results clearly evidence that the intense molecular-like resonances dominate in the near edge X-ray absorption of SF₆-clusters and solid SF₆. There are, however, substantial differences. Firstly, the experimental redshifts of the S 2p^{1/2}t_{2g} and 2p^{1/2}e_g shape resonances in clusters 35 ± 5 meV and 95 ± 5 meV increase to 90 ± 10 meV and 320 ± 10 meV in solid SF₆. No visible shifts are revealed for the lowest S 2p^{1/2}a_{1g} resonance. Similar spectral shifts are observed for the F 1s-regime. Secondly, the relative intensities of the core-to-valence excitations are subject of substantial changes in clustered and solid SF₆. Thirdly, new spectral features are observed in solid SF₆. Their origin is discussed. The DBOP model is applied to rationalize and compute the shifts of the core-to-valence excitations in SF₆ clusters and condensed SF₆. The influence of chemical bonding, dynamic stabilization, intra- and intermolecular motions, multiple scattering and multi-electron excitations on the spectral shifts, as well as changes in the intensities of the molecular excitations and the occurrence of new spectral features in condensed SF₆ is discussed.

5P078

Cu-ZnO@C nanoreactors studied by in-situ synchrotron SAXS spectroscopyCI Hong,¹ HY Kang,¹ HP Wang,¹ US Jeng,² CH Su²¹Department of Environmental Engineering, National Cheng Kung University, Tainan, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan

In core-shell nanoreactors, enhanced partial oxidation of methanol (POM) at relatively low temperatures may occur. The changes of electronic density of the catalytic active species can be observed by small angle X-ray scattering (SAXS) spectroscopy. An in-situ synchrotron SAXS has, therefore, been used to study nanostructure of Cu-ZnO encapsulated in the porous carbon shell (Cu-ZnO@C) during temperature-programmed carbonization at the temperature range of 323-523 K. The in-situ SAXS spectra show that the Cu-ZnO@C behaviors like a nanoreactor for catalytic POM to yield H₂. The active species (Cu) may be partially oxidized to higher oxidation states during POM at the temperature of <453 K.

5P079

Evolution of metallic screening within the sub-nm rangeM Neeb,¹ S Peters,¹ S Peredkov,¹ W Eberhardt¹¹Helmholtz-Zentrum Berlin, Wilhelm-Conrad-Röntgen-Campus Adlershof (BESSY II), Berlin, Germany

Auger spectra of small copper clusters supported by a thin silica layer have been measured as function of cluster size. The Auger kinetic energy of the nanoclusters clearly changes with the excess energy of the emitted photoelectron. The energy shift exhibits a reduced metallic screening ability of small clusters with respect to the bulk for which the Auger energy does not depend on the excitation energy. The spectroscopic data reveal an evolution from a long-range Coulomb-like interaction to a short-range "screened" electrostatic interaction within the sub-nm range. The attenuated electrostatic screening ability of the supported metal clusters with a radius <1 nm should have consequences for important properties such as catalysis involving charge transfer, conductivity and electron correlation.

5P081

The radiation-induced copper nanoclusters: XANES and DFT studyVL Mazalova,¹ AV Soldatov,¹ RA Mayanovic²¹Center for Nanoscale Structure of Matter, Southern Federal University, Rostov-on-Don, Russian Federation; ²Missouri State University, Springfield, United States

Synchrotron radiation is a powerful tool for an operated nanoclusters growth using radiolysis process and at the same time for their *in situ* investigation. Traditionally the pulse radiolysis is a technique for the elucidation of a variety of inorganic reaction mechanisms, especially in aqueous solutions. This technique is based on the formation of the radicals e_{aq}⁻, H, and OH by the radiolysis of water. We have shown that irradiation of copper (II) chloride in aqueous solutions by synchrotron radiation in the absence of any stabilizer leads to the synthesis of metal nanoparticles. Moreover, X-rays used for the synthesis allow simultaneous *in situ* study of copper nanoparticles formation by X-ray absorption spectroscopy. The changes of atomic structure and chemical bonding were simultaneously monitored by means of X-ray absorption fine structure (XAFS) spectroscopy. XAFS analysis allows obtaining the detailed information on local and electronic structure with high sensitivity. Research objective of the copper nanoclusters obtained as a result of a radiolysis is study of a geometrical structure of clusters during of their growth using XAFS analysis and also an explanation of the energy shift of the XAFS spectra for clusters of different sizes. The theoretical analysis of X-ray absorption spectra were performed by the full-potential finite-difference approach and using optimized geometries calculated by the all-electron density functional theory. In the present work is shown that at initial stage the copper clusters grow in the structure which is different from the bulk copper. Part of the research (A.V.S. and V.L.M.) has been supported by Russian Foundation for Basic Research, Grant No. RFBR 09-02-12257-ofi_m.

5P082

Ultra-fast dynamics of spin and orbital magnetic moments by time resolved XMCD.

C Boeglin,¹ E Beaurepaire,¹ V Halté,¹ V Lopez-Flores,¹ J Arabski,¹ C Stamm,² N Pontius,² HA Dürr,² JY Bigot¹

¹Institut de Physique et de Chimie de Strasbourg, UMR7504, CNRS et Université de Strasbourg, Strasbourg, France; ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, Berlin, Germany

Ultrafast magnetization dynamics is an important issue for both fundamental science and for applications. Since the first observation of laser induced spin dynamics, the mechanisms of angular momentum dissipation at picosecond timescales have been debated and in order to discuss such microscopic mechanisms, it is desirable to quantitatively probe absolute values of magnetization with high temporal resolution. In this context, we have used ultrashort optical laser pulses (60 fs duration) to induce changes of the magnetization in a ferromagnetic CoPd alloy film with perpendicular anisotropy; the dynamics was probed with circularly polarized femtosecond X-ray pulses (100 fs duration), measuring the X-ray magnetic circular dichroism (XMCD) at Co L₂ and L₃ edges. The use of sum rules of XMCD allows disentangling for the first time, the spin and orbital components of the magnetic moment. We show that the dynamics of L_z and S_z are different, leading to a drop by ~30% of the ratio L_z/S_z about 500 fs after the absorption of the laser pulse. These signals will be compared to the purely electronic effect, measured by the intensity at L₃ edge with linearly polarized X-rays. Our results show that the mechanism responsible for the ultrafast laser induced demagnetization requires the concept of spin-orbit interaction, and that the magneto-crystalline anisotropy energy is an important quantity to consider.

5P083

Mechanistic studies of the dissociative photoionization of 1,3-butadiene

W Fang,¹ L Gong,¹ X Shan,¹ F Liu,¹ Z Wang,² L Sheng¹

¹National synchrotron radiation laboratory School of Nuclear Science and Technology University of Science and technology of China , Hefei, Anhui, China; ²Laboratory of Environmental Spectroscopy, Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui, China

VUV dissociative photoionization of 1,3-butadiene in a region ~8.5–17 eV is investigated with photoionization mass spectrometry (PIMS) using tunable VUV synchrotron radiation (SR). The ionization energy (IE) of 1,3-butadiene and appearance energies (AEs) for its fragment ions, C₄H₅⁺, C₄H₄⁺, C₄H₃⁺, C₃H₃⁺, C₂H₄⁺, C₂H₃⁺, C₂H₂⁺, were observed at 9.09, 11.73, 13.13, 15.17, 11.52, 12.51, 15.20 and 15.22 eV, respectively. The IE of C₄H₆ and the AEs of its main fragments are calculated with G2 and G3B3 methods using Gaussian 03 suite of programs. Based on comparison of determined appearance energies and energies predicted with the ab initio calculations, seven dissociative photoionization channels are proposed: C₄H₅⁺ + H, C₄H₄⁺ + H₂, C₄H₃⁺ + H₂ + H, C₃H₃⁺ + CH₃, C₂H₄⁺ + C₂H₂, C₂H₃⁺ + C₂H₂ + H, and C₂H₂⁺ + C₂H₂ + H₂. C₃H₃⁺ + CH₃ is found to be the dominant channel, followed by C₄H₅⁺ + H and C₂H₄⁺ + C₂H₂.

5P084

Dynamic investigation of photoinduced phase transition in Prussian blue analogs by picosecond time-resolved XAFS

S Nozawa,¹ T Sato,¹ A Tomita,² M Hoshino,² H Tokoro,³ S I Ohkoshi,³ S Y Koshihara,² S I Adachi¹

¹High Energy Accelerator Research Organization, Institute of Materials Structure Science, Tsukuba, Ibaraki, Japan; ²Department of Materials Science, Tokyo Institute of Technology, Meguro-ku, Tokyo, Japan; ³Department of Chemistry, School of Science, The University of Tokyo, Bunkyo-ku, Tokyo, Japan

Prussian blue analogs have recently attracted great interest due to their exotic natures such as photo-magnetization as well as photo-structural change in the photoinduced phase transition (PIPT).^{1,2} The investigation of the dynamics of PIPT allows us to obtain information how the photo-excitation in the single site expands into a macroscopic phase transition. Picosecond time-resolved XAFS experiments were performed on the NW14A at the Photon Factory Advanced Ring (PF-AR).^{3,4} The time-resolved XAFS spectra were collected by the pump and probe technique combined with a femtosecond laser system. In EXAFS and XANES regions, spin-lattice-charge coupled dynamics accompanied with the PIPT were obtained at 100 ps resolution. The detailed results will be presented.

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5P085

Dynamic study of electronic properties of photoactive Eu^{3+} complexes thin film on gold(111)

MG Silly,¹ C Chauvet,¹ F Sirotti,¹ F Charra,² F Lux,³ G Lemerrier⁴

¹TEMPO Beamline, Synchrotron SOLEIL, Gif-Sur-Yvette, France; ²Service Laboratoire d'Electronique et nanoPhotonique Organique, DSM/IRAMIS/SPCSI/LEPO, CEA Saclay, Gif-Sur-Yvette, France; ³Laboratoire de Physico-Chimie des Matériaux Luminescents (LPCML), Villeurbanne, France; ⁴Université Reims Champagne-Ardenne, CNRS 6229, ICMR ; Groupe Chimie de Coordination, Reims, France

Luminescence of transition metal compounds driven by external stimuli is of great interest in the development of photonic materials for use as molecular memories, switches or sensors. Lanthanide ion complexes are photoactive species showing potential applications in light conversion molecular devices. Actually, the use of Lanthanide ion complexes involving π -conjugated ligands overcomes the very small absorption coefficient at UV wavelength of isolated lanthanide ions, by energy transfer processes. Playing the part of antenna, the ligands absorb the exciting light and after internal intersystem crossing from singlet to triplet state, transfer their energy to the lanthanide ion which subsequently de-excites radiatively. In order to determine the different electronic states and chemical species involved in excitation/de-excitation processes of Eu^{3+} complexes, and to avoid substrate/molecular complexes interactions, we have performed a complete study of electronic properties of $\text{Eu}(\text{DYP})_2\text{Cl}_3$ thin film on gold (111) by mean of core level and resonant photoemission spectroscopies. Time resolved pump/probe (LASER/SR) experiments using a photoelectron energy analyser equipped with a fast delay line detection system showed that deexcitation processes are dominated by charging effects with a decay time in the hundred of milliseconds range.

5P086

Excited-electron dynamics of bismuth film grown on Si (111) surface by interferometric time-resolved two-photon photoelectron spectroscopy

S Fujimasa,¹ M Imamura,² H Yasuda³

¹Department of Mechanical Engineering, Kobe University, Nada, Kobe, Japan; ²Synchrotron Light Application Center, Saga University, Saga, Saga, Japan; ³Research Center for Ultra-High Voltage Electron Microscopy, Osaka University, Ibaraki, Osaka, Japan

Bismuth is a typical semi-metallic element and various studies on the relevant characteristic properties have been carried out for the purpose of applications to electronic, optic and magnetic devices. From viewpoints of device applications and fundamental physics, photo-excited electrons play an important role in physical and chemical phenomena and it is necessary to understand the carrier dynamics. We have carried out a femtosecond interferometric time-resolved two-photon photoemission (ITR-2PPE) study in order to investigate the excited electron dynamics on femtosecond time-scale at excited states of bismuth film on Si (111) surface. Two kinds of crystalline bismuth films were prepared by vapor-deposition onto an Si (111) 7×7 clean surface (p-type 0.02 Ωm wafer) using Knudsen-cell. On the single crystalline Bi (111) surface, all the energy relaxation time of excited-electron is less than 15 fs in the energies (E_i) of the range from 1.0 to 2.6 eV above Fermi energy, and decreases with increasing E_i . This result indicates that this fast relaxation is induced by electron-electron scattering. The values of the energy relaxation time measured can be described as a function of $9.15 \times E_i^{-1.10}$. On the other hand, on the poly crystalline Bi surface, the values of the energy relaxation time by electron-electron scattering are slightly larger than those on the single crystalline surface, and can be described as a function of $11.41 \times E_i^{-0.75}$. That means the electron-electron scattering rate of single crystalline bismuth surface is higher. It is suggested that the single crystalline bismuth surface has higher densities of states near the Fermi surface than those of poly crystalline bismuth surface, since excited electron is necessary to scatter with valence band electrons under the condition of both energy and momentum conservation.

5P087

Studies of chemical reactions $\text{O}(^3\text{P}/^1\text{D}) + \text{C}_2\text{H}_4/\text{C}_2\text{H}_3\text{F}$ using undulator radiation as an ionization source

SH Lee,¹ WK Chen,¹ WJ Huang¹

¹Scientific Research Division, National Synchrotron Radiation Research Center, Hsinchu, Taiwan

We conduct the reactions of ^3P and ^1D oxygen atoms with ethylene (C_2H_4) and vinyl fluoride ($\text{C}_2\text{H}_3\text{F}$) in a crossed-molecular-beam time-of-flight apparatus using selective photoionization. Two oxygen-atom sources that have the same velocity distributions but different $^3\text{P}/^1\text{D}$ electronic-state distributions are employed to disentangle reaction products from the two atomic oxygen reactants. In the reactions of $\text{O}(^3\text{P}/^1\text{D}) + \text{C}_2\text{H}_4/\text{C}_2\text{H}_3\text{F}$, product $\text{C}_2\text{H}_3\text{O}/\text{C}_2\text{H}_2\text{FO} + \text{H}$ arises from the reaction of ^3P oxygen atoms alone but product $\text{CH}_3/\text{CH}_2\text{F} + \text{HCO}$ arises from reactions of oxygen atoms in both ^3P and ^1D states. Product $\text{C}_2\text{H}_3\text{O}$ ($\text{C}_2\text{H}_2\text{FO}$) is scattered preferentially into the backward hemisphere, indicating a direct reaction on the triplet potential-energy surface involving no persistent reaction complex. The excitation function of product $\text{C}_2\text{H}_3\text{O}$ ($\text{C}_2\text{H}_2\text{FO}$) indicates a collision-energy threshold of 1.2 (2.2) kcal mol⁻¹ corresponding to an entrance barrier in the reaction $\text{O}(^3\text{P}) + \text{C}_2\text{H}_4$ ($\text{C}_2\text{H}_3\text{F}$). In contrast, product CH_3 (CH_2F) + HCO is scattered equivalently into the forward and backward hemispheres, indicating that the reactions of oxygen atoms either in state ^3P or ^1D involve persistent reaction complexes. Reactions of both ^3P and ^1D oxygen atoms with ethylene are responsible also for the production of $\text{CH}_2\text{CO} + \text{H}_2$. Furthermore, atomic $\text{O}(^1\text{D})$ is 40–90 times the reactivity of atomic $\text{O}(^3\text{P})$ in reactions with ethylene and vinyl fluoride.

5P088

Resonance photoelectron-recoil-induced rotational excitation of the $B^2\Sigma_u^+$ state in N_2^+ at the $1\sigma_u \rightarrow 1\pi_g$ resonance

YS Krivosenko,¹ AA Pavlychev,¹ J Plenge,² M Meyer,³ E Ruehl²¹Department of Physics, St. Petersburg State University, St. Petersburg, Russian Federation; ²Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Berlin, Germany; ³ISMU, Centre Universitaire Paris-Sud, Orsay, France

Rotational heating of the molecular ion increases with kinetic energy of the ejected electron. This is evidenced by recent photoelectron and fluorescent decay studies of the $B^2\Sigma_u^+$ state in N_2^+ . Special emphasis is put on photoelectron-recoil-induced rotational excitation of the $B^2\Sigma_u^+$ state in N_2^+ in the vicinity of the intense $1\sigma_u \rightarrow 1\pi_g$ excitation, which is observed in N_2 400.84 eV photon energy. Changes in rotational energy ΔE as a function of excitation energy are examined using the VDFN model in order to take the zero-point vibrational motion into account. The calculations evidence a linear spectral dependence of ΔE below the $1\sigma_u \rightarrow 1\pi_g$ transition. An increase of the rotational excitation of the $B^2\Sigma_u^+$ state in N_2^+ is observed at 400.84 eV. The computed sharp increase $\Delta E \approx 1$ meV is associated with the ro-vibration interaction and population of highly-excited vibrational levels in the intermediate $N_2^+(1\sigma_u^{-1}\pi_g^1)$ state. Rotationally resolved measurements of the fluorescence decay of the $B^2\Sigma_u^+$ state in N_2^+ are carried out in the π_g^* -resonance regime. These results confirm the resonance behavior of the rotational excitation of the $B^2\Sigma_u^+$ state in N_2^+ and highlight the increase of the rotational excitation of ≈ 6 meV at the $1\sigma_u^{-1}\pi_g^1$ resonance. Plausible reasons of the giant enhancement of the N_2^+ rotations at 400.84 eV are discussed.

5P089

A modest size X-ray free-electron laser

TY Lee,¹ HS Kang²¹Beamline Department, Pohang Accelerator Laboratory, Pohang, Kyungbuk, Republic of Korea;²Accelerator Department, Pohang Accelerator Laboratory, Pohang, Kyungbuk, Republic of Korea

X-ray free-electron laser (XFEL) machines are all so huge in size that it looks almost impossible to have this facility in our neighborhood. This paper shows how the XFEL size depend upon relevant physical parameters. It is argued that the XFEL size can be reduced considerably to a modest size by designing carefully.

5P090

The JLamp VUV/soft X-ray user facility

GR Neil,¹ GP Williams,¹ F Team¹¹Jefferson Laboratory, NewportNews, VA, United States

Jefferson Lab (JLab) is proposing JLAMP (JLab AMplifier), a 4th generation light source covering the range 10–100 eV in the fundamental mode with harmonics stretching towards the oxygen k-edge. The scientific purpose is to study ultrafast dynamics in complex systems as a pathway to the understanding and creation of novel materials and devices, with a twin focus on changing our approach to the use of energy and on improving our stewardship of the environment. Expert groups of physicists and chemists have identified the game-changing science offered by such a light source. The machine will be based on an energy upgrade to an existing energy-recovering linear accelerator at JLab, made possible by advances in superconducting accelerator technology. Specifically, accelerating gradients of 20 MV/m and electron-beam recirculation will allow electron-beam energies of >600 MeV to be achieved at repetition rates up to 4.68 MHz with continuous wave RF. The average brightness will substantially exceed existing light sources in this device's wavelength range of 100 nm down to 10 nm, extended by harmonics towards 2 nm. Multiple photon sources will be made available for pump-probe dynamical studies. The system will be capable of operating as a seeded amplifier for precise pulse length and bandwidth control or as an oscillator at higher average brightness. The plans for construction of this User facility will be presented. We will also present an overview of the science case supporting the submission.

5P091

Three-photon double ionization of Ar^+ by extreme ultraviolet free-electron laser: manifestation of intermediate resonances of Ar^+

N Miyauchi,^{1,5} J Adachi,^{1,5} A Yagishita,^{1,5} T Sako,² F Koike,³ T Sato,^{4,5} A Iwasaki,^{4,5} K Yamanouchi,^{4,5} M Nagasono,⁵ K Tono,⁵ M Yabashi,⁵ T Ishikawa,⁵ T Togashi,^{5,6} H Ohashi,^{5,6} H Kimura,^{5,6} Y Senba^{5,6}¹Photon Factory, Institute of Materials Structure Science, KEK, Tsukuba, Ibaraki, Japan; ²College of Science and Technology, Nihon University, Funabashi, Chiba, Japan; ³School of Medicine, Kitasato University, Sagami-hara, Kanagawa, Japan; ⁴School of Science, The University of Tokyo, Bunkyo, Tokyo, Japan; ⁵RIKEN, XFEL Project Head Office, Sayo, Hyogo, Japan; ⁶Japan Synchrotron Radiation Research Institute, Sayo, Hyogo, Japan

Three-photon double ionization of Ar atom has been investigated by photoelectron spectroscopy using extreme ultraviolet free-electron laser of the Spring-8 Compact SASE Source. When the photon energy of the laser has been tuned to the intermediate 3p-3d and 3p-4d resonances of the Ar^+ ion, photoelectron peaks due to two-photon single ionization of Ar^+ ion have been observed for the first time. And it has been revealed that the appearance of the peaks is controlled by the mixing coefficients of multi-configurations describing the intermediate resonance states. Furthermore, it has been shown that in the region $< 2.2 \times 10^{13} \text{ W/cm}^2$, the laser intensity dependence of the Ar^{2+} ion production rate due to the two-photon single ionization strongly deviates from that expected from first-order perturbation theory.

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Simulations on ultraviolet short pulse free-electron lasers at perfect synchronism

Y Dou,¹ X Shu¹¹Institute of Applied Physics and Computational Mathematics, Beijing, China

It is proposed that an ultraviolet ultra-short pulse can be generated using a free-electron laser (FEL) at perfect synchronism. Three-dimensional simulations and theoretical analyses on ultraviolet short FEL pulse at perfect synchronism are carried out using our 3D OSIFEL code. These studies include the development of optical field and the evolution of the optical pulses at detuning length of the cavity is zero. The numerical simulations confirm that the optical pulse centroid is retarded on successive passes due to the slippage between the optical and electron beams and an ultra-short optical pulse is finally formed in an FEL oscillator at the perfect synchronism.

5P093

Chirped pulse amplification in a single pass free-electron laser amplifier

X Shu,¹ T Peng,² Y Dou¹¹Institute of Applied Physics and Computational Mathematics, Beijing, China; ²School of Physics and Technology, Wuhan University, Wuhan, China

Linear chirped pulse amplification at single pass free-electron laser (FEL) amplifier is studied through numerical simulations. The processes of chirped pulses with different chirped parameters being amplified by the FEL amplifier or the FEL amplifier with energy-chirped electron beam are studied. The peak power and width of the final compressed pulse with different chirped parameters have been calculated. The results show that, the FEL amplifier can amplify the chirped pulse, the peak power of the final compressed pulse can reach 10s GW and the width of the pulse can be 10s fs with the parameters of TTF. In the case of using the energy-chirped electron beam to amplify chirped pulse, the gain bandwidth of the FEL amplifier will be wider and the chirped parameter will be larger more. The peak power of the final compressed pulse can even reach near 10 times larger and the width of the pulse 10 times shorter than that with normal electron beam.

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Terahertz-field driven streak-camera for single-shot measurements of the temporal profile of XUV-pulses from FLASH

U Frühling,¹ M Gensch,² T Gebert,¹ B Schütte,¹ R Kalms,¹ M Krikunova,¹ E Ploenjes,³ M Drescher¹¹Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany; ²Helmholtz-Zentrum Berlin, Berlin, Germany; ³Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

The Free-Electron Laser in Hamburg (FLASH) delivers highly intense ultrashort XUV light pulses with pulse durations of a few femtoseconds. Due to the stochastic nature of the light generation scheme based on self amplified spontaneous emission (SASE), the duration and temporal profile of the XUV pulses fluctuate from shot to shot. For a single shot measurement of the temporal profile a THz-field driven streak-camera has been developed. In the experiment the XUV pulses are superimposed in a gas target with synchronized THz-pulses generated by the same electron bunch in a THz-undulator downstream of the SASE XUV-undulator. The XUV photons ionize the gas atoms and generate photoelectrons. These photoelectrons are accelerated by the time-dependent electric field of the THz-light pulse, where the momentum gain depends on the THz electric field at the ionization time. By measuring the photoelectron momenta we can therefore reconstruct the temporal profile of the ionizing XUV pulse. This technique is intensively used in attosecond metrology where near infrared streaking fields are employed. Here, it is adapted for the analysis of pulse durations in the few femtosecond range by choosing a hundred times longer far infrared streaking wavelength.

5P095

Angular distribution anisotropy parameters of sequential and simultaneous few-photon double ionization

M Braune,¹ A Reinköster,¹ S Korica,¹ J Viefhaus,² U Becker^{1,3}¹FHI der MPG, Berlin, Germany; ²DESY, Hamburg, Germany; ³KSU, Riyadh, Saudi Arabia

Using angle-resolved photoelectron spectroscopy in experiments at the FLASH facility we were able to distinguish various sequential and simultaneous pathways of few-photon double-ionization of rare gases. The results show that sequential double-ionization is the dominant process if the required threshold is exceeded by the photon energy. The photoelectron angular distributions of these two-photon processes differ from a distribution of a dipole transition showing contributions of higher order Legendre polynomials. Values of the corresponding higher order anisotropy parameter β_4 could be determined and compared to recent calculations [1, 2]. Especially for argon and krypton, the calculations predict a dramatic change in the β_4 -values at a photon energy around 50eV and 80eV, respectively, due to the Cooper minimum in the cross section. Surprisingly, in this energy range the β_4 -values depend strongly on the coupling of the ionic final states although the Cooper minimum is basically a radial effect due to the changing overlap of the wavefunctions of the bound and the outgoing electron with increasing energy. This is a clear signature of differences in the anisotropic interactions in the final state of the photoelectron and the ionic core depending on the angular momentum coupling of the ionic terms. Our data give first evidence for this effect in argon for the ³P, ¹S and ¹D doubly charged final ionic states. A substantial variation of β_4 is also observed in the preliminary data analysis of the sequential double ionization of krypton.

[1] A.S. Kheifets, J. Phys. B **40**, F313 (2007) [2] S. Fritzsche *et al.*, J. Phys. B **41**, 165601 (2008)

5P096

Pulse energy measurement of an extreme-ultraviolet free-electron laser using a cryogenic radiometer

M Kato,^{1,2} N Saito,^{1,2} PN Juranić,^{2,3} M Richter,^{2,4} AA Sorokin,^{2,3,4,5} K Tiedtke,^{2,3} Y Morishita,¹ T Tanaka,^{1,2} U Jastrow,³ U Kroth,⁴ H Schöppe,⁴ M Nagasono,² M Yabashi,² K Tono,² T Togashi,^{2,6} H Kimura,⁶ H Ohashi,⁶ T Ishikawa²

¹AIST, NMIJ, Tsukuba, Japan; ²RIKEN, XFEL Project Head Office, Sayo, Hyogo, Japan; ³DESY, Hamburg, Germany; ⁴PTB, Berlin, Germany; ⁵Ioffe Physico-Technical Institute, St Petersburg, Russian Federation; ⁶JASRI, Sayo, Hyogo, Japan

We measured the absolute single-shot pulse energy of an extreme-ultraviolet free electron laser (EUV-FEL) using a cryogenic radiometer which is used as the primary standard instrument for measuring the absolute intensity of monochromatized soft X-rays in the National Metrology Institute of Japan (NMIJ). The experiment was performed using the SCSS test accelerator EUV-FEL located at Spring-8. A gas monitor detector developed by Physikalisch-Technische Bundesanstalt (PTB)/ Deutsches Elektronen-Synchrotron (DESY)/ Ioffe Physico-Technical Institute (Ioffe) was set up in front of the radiometer so that the pulse energy could be measured with both detectors. The results obtained with the two different detectors agree within 2.0 %, which is well below their combination relative standard uncertainty of 5.9 %.

5P097

Comparison for measuring the absolute radiant power of an extreme-ultraviolet free-electron laser between a gas monitor detector and a cryogenic radiometer

M Kato,^{1,2} PN Juranić,^{2,3} M Richter,^{2,4} N Saito,^{1,2} AA Sorokin,^{2,3,4,5} K Tiedtke,^{2,3} U Jastrow,³ U Kroth,⁴ H Schöppe,⁴ M Nagasono,² M Yabashi,² K Tono,² T Togashi,^{2,6} A Higashiya,² H Kimura,⁶ H Ohashi,⁶ T Ishikawa¹

¹AIST, NMIJ, Tsukuba, Japan; ²RIKEN, XFEL Project Head Office, Sayo, Hyogo, Japan; ³DESY, Hamburg, Germany; ⁴PTB, Berlin, Germany; ⁵Ioffe Physico-Technical Institute, St Petersburg, Russian Federation; ⁶JASRI, Sayo, Hyogo, Japan

We performed a comparison measurement for the absolute radiant power of an extreme-ultraviolet (EUV) free electron laser (FEL) between a gas monitor detector (GMD) developed by Physikalisch-Technische Bundesanstalt (PTB) / Deutsches Elektronen-Synchrotron (DESY) / Ioffe Physico-Technical Institute (Ioffe) and a cryogenic radiometer of National Institute of Advanced Industrial Science and Technology (AIST). Using the SCSS test accelerator EUV-FEL located at Spring-8, the measurements were performed at the wavelengths of 51.3, 56.1 and 61.2 nm and at the repetition of 20 Hz. The results obtained with the GMD and the radiometer agree within 2.6 % which is less than their combination relative standard uncertainty, which varies from 4.1 % to 5.5 %.

5P098

Correlated measurements of fluorescence and ion spectra after X-FEL ionization of Ne and Xe

B Rudek,^{1,8} D Rolles,^{1,7} A Rudenko,^{1,8} S Epp,^{1,8} L Foucar,^{1,7} B Erk,^{1,8} R Hartmann,^{1,2} N Kimmel,² C Reich,² P Holl,² L Strueder,^{1,2} H Hirseman,³ C Bostedt,⁴ J Bozek,⁴ J Schulz,⁵ L Gumprecht,⁵ A Aquila,⁵ N Rohringer,⁶ K U Kuehnel,⁸ J Ullrich^{1,8}

¹Max Planck Advanced Study Group at CFEL, Hamburg, Germany; ²Max Planck Semiconductor Lab, München, Germany; ³DESY, Hamburg, Germany; ⁴LCLS, Menlo Park, United States; ⁵CFEL, Hamburg, Germany; ⁶LLNL, Livermore, United States; ⁷Max-Planck-Institute for Medical Research, Heidelberg, Germany; ⁸MPI for Nuclear Physics, Heidelberg, Germany

User assisted commissioning has recently started at the world's first X-ray free electron laser (FEL), the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory in Stanford. LCLS provides unprecedented ultra-intense X-ray radiation, in which light-matter interaction is dominated by multiphoton absorption processes. Thus for noble gas targets, calculations [Rohringer, Phys. Rev. A 76, 033416] predict the formation of extremely high charge-states by a sequence of photoionization and Auger decay. The higher the charge state, however, the higher the probability of fluorescence decay over Auger decay. We have investigated the competition between Auger and fluorescent decay in highly charged neon (up to 10+) and xenon (up to 35+) by means of correlated ion time-of-flight and fluorescence spectroscopy. The fluorescence yield has been found to be increased for higher charge states of neon; Xenon shows enhanced fluorescence when the M shell becomes depleted.

5P099

Towards water window harmonics generated with a novel 1.8 μm sub two cycle laser source

F Légaré,¹ BE Schmidt,^{1,2} AD Shiner,^{2,3} M Giguère,¹ C Trallero-Herrero,³ DM Villeneuve,³ JC Kieffer,¹ PB Corkum^{2,3}

¹INRS-EMT, Varennes, QC, Canada; ²University of Ottawa, Ottawa, ON, Canada; ³National Research Council, Ottawa, ON, Canada

High harmonic generation (HHG) is the key process to generate attosecond laser pulses. Recently, isolated 80 attosecond pulses have been generated using 1.5 cycle carrier envelope phase stabilized 800 nm laser pulses [1]. Further shortening of attosecond pulse duration utilizing HHG can be achieved by using few cycle pulses at longer wavelengths of the driving laser because the cut-off shifts towards higher photon energies proportional to λ^2 . A simple scheme for generating sub mJ sub two cycle pulses at 1.8 μm (1 cycle = 6 fs) is presented [2]. Optical parametric amplified pulses are spectrally broadened in a hollow-core fiber filled with Argon and subsequently compressed by utilizing linear propagation through bulk material. The physical mechanism of this robust pulse compression approach and its spectral tunability in the mid-IR will be described with numerical simulations of nonlinear propagation in the hollow-core fiber. Using Argon as the gas media and an intensity of $\sim 3 \times 10^{14}$ W/cm², HHG spectra extending up to ~ 5 nm wavelength (240 eV) photons have been generated. Scaling up the intensity of the infrared sub two cycle laser source as well as getting shorter wavelength X-rays (~ 1 nm) using HHG from neon and helium will be discussed.

[1] E. Goulielmakis et al. Single-cycle nonlinear optics, *Science* **320**, 1614-1617 (2008).

[2] B. E. Schmidt et al. Compression of 1.8 μm laser pulses to sub two optical cycles with bulk material, accepted at *App. Phys. Lett.* (2010).

5P100

Performance of a polarizer using synthetic mica for the 12-25 nm wavelength range

M Cui,¹ K Chen,¹ J Zhao,² L Sun,¹ S Xi,¹ F Yan¹

¹BSRF, Institute of High Energy Physics, CAS, Beijing, China; ²School of Mechanical Engineering, Beijing Technology and Business University, Beijing, China

To develop the polarizer functioning in the extreme ultraviolet (EUV) and soft X-ray region from 12-25nm, a polarization performance of synthetic mica has been investigated theoretically with a simulation code using Fresnel equations and optical constants from Henke database. The reflectance of synthetic mica crystal for s and p polarization was measured to investigate its polarization performance in a home-made synchrotron radiation soft X-ray polarimeter at beamline 3W1B, Beijing Synchrotron Radiation Facility (BSRF). The reflectivity of the synthetic mica crystal at the angle of grazing incidence of 48° were obtained from the experimental data, which are about 4.8×10^{-3} at 25nm and 6.0×10^{-4} at 12nm, and the linear polarizance of the X-ray reflected by the synthetic mica crystal we measured using an analyzer-rotating method increases from 80% to 96.6% in this soft X-ray region, while higher than 98.2% in the simulation. The result indicates that this synthetic mica crystal works as a practical polarizer in this EUV and soft X-ray region of 12-25nm, and also extensive wavelength region high than 25nm.

5P101

A novel 3D ARPES electron spectrometer for pulsed photon sources

R Moberg¹

¹VG Scienta AB, Uppsala, Sweden

In this presentation we report on the continued development of the ARTOF 10k, a novel 3D ARPES instrument for electron spectroscopy dedicated for pulsed photon sources. This new spectrometer is based on the time of flight principle but is combined with a lens system in order to increase the acceptance angle, and conserve the angular information of the photoemission in a full $\pm 15^\circ$ cone, allowing high precision ARPES and large solid angle transmission measurements. Recent experimental results from different customer set-ups prove that the ARTOF 10k is an efficient research tool compatible with photon source repetition rates from the few kHz range up to 3 MHz. This makes the spectrometer suitable for a wide range of photon sources such as lasers and synchrotrons in special bunch modes. The presentation will also contain results exemplifying that the ARTOF 10k can be run in remote control mode (external software communication).

5P102

Compact light source with single bend lattice

TY Lee¹

¹Beamline Department, Pohang Accelerator Laboratory, Pohang, Kyungbuk, Republic of Korea

To construct a compact light source with as many as possible insertion devices, a lattice is proposed to have a single bending magnet in a cell. It accommodates twice as many insertion devices as the usual double bend lattice, while the performance is almost the same.

5P103

Status of the metrology light sourceR Klein,¹ R Thornagel,¹ G Ulm,¹ J Feikes,² G Wüstefeld²¹Physikalisch-Technische Bundesanstalt, Berlin, Germany; ²Helmholtz-Zentrum Berlin, Berlin, Germany

The Physikalisch-Technische Bundesanstalt (PTB), the German national metrology institute, has set up in close cooperation with the Helmholtz-Zentrum Berlin (HZB, formerly BESSY) the 630 MeV electron storage ring Metrology Light Source (MLS) [1]. This new electron storage ring is in regular user operation since April 2008 and is dedicated to synchrotron-radiation-based metrology and technological developments in the far-IR/THz, IR, UV, VUV and EUV spectral range. Of special importance for PTB is the operation of the MLS as a primary radiation source standard from the near IR up to the soft X-ray region. Moreover, as a dedicated THz storage ring source the MLS can be operated in a special low-alpha mode based on an octupole correction-scheme for the generation of short electron bunches. In this mode, the MLS delivers radiation in the far-IR/THz spectral range with enhanced intensity as compared to the normal mode of operation [2]. Several beamlines are in operation or under construction, including one undulator beamline, bending magnet beamlines for the calibration of radiation sources and detectors, an EUV metrology beamline and several IR/THz beamlines [3].

[1] R. Klein et al., Phys. Rev. ST-AB 11, 110701 (2008).

[2] R. Müller et al., AIP Conf. Proc. 1214, 32 (2010).

[3] R. Klein et al., Metrologia 46, S266 (2009).

5P104

A novel laser-plasma-source for the 1 keV regionI Mantouvalou,¹ T Bidu,¹ R Jung,² H Legall,² H Stiel,² W Malzer,¹ B Kanngiesser¹¹Institute for Optic and Atomic Physics, Technical University of Berlin, Berlin, Germany; ²Max-Born-Institute, Berlin, Germany

The concept of hitting a target with a focused, short-pulse, high average power laser beam in order to obtain tailored X-ray pulses has been introduced during the last two decades. Due to recent improvements in high average power solid state lasers producing short pulses in the ns or sub-ns range, laser induced plasmas covering a broad range of photon energies in the soft and hard X-ray region are nowadays used as laboratory X-ray sources. Up until now the main focus in the soft X-ray region has been laid on X-ray sources for extreme ultraviolet (EUV)-lithography at 13.5 nm and X-ray sources in the water window (2.3 – 4.4 nm) for the analysis of biological samples. In this contribution we describe the concept of a laser-plasma-source (LPS) for the 1 keV region. A stable laser-plasma-source in the 1 keV region is especially interesting for the investigation of L-edges of transition metals, thus, enabling analysis of technological samples with a depth resolution in the nm-regime. The lack of suitable X-ray tubes in this energetic region and factors like beam time restrictions at synchrotron sources will render this new instrument into a valuable tool for X-ray spectroscopy. The concept of our LPS is based on a high average power commercial Yb:YAG – disk laser system (TRUMPF Laser Technology) which was modified with a 1 ns seed-diode in order to obtain optimal pulse parameters. First X-ray spectra and photon yield calculations will be presented as well as investigations concerning the optimal target material.

5P105

Extremely low energy high resolution photoemission system using electron-cyclotron resonance plasma discharge emission linesL Plucinski,¹ S Suga,^{1,2} P Baltzer,³ CM Schneider¹¹Institut f. Festkörperforschung IFF-9, Forschungszentrum Jülich, Jülich, Germany; ²Graduate School of Engineering Science, Osaka University, Osaka, Japan; ³MB Scientific AB, Uppsala, Sweden

An extremely low energy photoemission system has been commissioned in the IFF-9 in FZ Jülich. A commercial electron-cyclotron resonance laboratory gas discharge source (from MB Scientific) has been customized for use with 3 gases (Xe, Kr, and Ar) in order to produce 3 discrete emission lines at 8.44, 10.03 and 11.62 eV each of the resolution below 1 meV [1]. Each gas requires its dedicated low-pass transmission filter (sapphire, CaF₂, and LiF) which removes the unwanted emission lines at higher photon energies, and furthermore the entire system of the light source is vacuum separated from the experimental chamber by the extra LiF window. For each gas certain extra lines do exist at lower photon energies, which might be both due to the gas itself and due to impurities. However, their influence is below the detection level for Xe, while Kr typically contains small amounts of Xe, which leads to the line of 0.3% relative intensity. For Ar there are clear extra lines which leave only approx. 1 eV of the energy below the Fermi level unaffected. We will present angle resolved photoemission data on Cu(111) and Fe/MgO(0001) systems on samples cooled to 90K. Clear dispersion of the Cu(111) surface state serves for calibration purposes, while the investigation of Fe/MgO(0001) presents the usefulness of our ELEPES system to investigate the interface states by utilizing the increased mean free path at lower electron kinetic energies.

[1] G. Funabashi, H. Fujiwara, A. Sekiyama, M. Hasumoto, T. Ito, S. Kimura, P. Baltzer, and S. Suga, Jpn. J. of Appl. Phys. **47**, 2265 (2008).

5P106

Optical-field-induced ionization vacuum ultraviolet laser at 126 nmS Kubodera¹, M Kaku¹, M Katto²¹Dept. of EEE, University of Miyazaki, Miyazaki, Japan; ²Cooperative Research Center, University of Miyazaki, Miyazaki, Japan

We have proposed and demonstrated an excitation method to realize a practical Ar₂* laser using optical-field-induced-ionization (OFI) electrons produced by a high-intensity femtosecond laser. The OFI electrons could be utilized to initiate the Ar₂* formation kinetics, since the initial plasma conditions through the OFI process can be controlled by the choice of high-intensity laser parameters such as polarization and intensities. In this abstract, we report the optical amplification characteristics of the OFI Ar₂* excimer VUV amplifier at 126 nm. An OFI Ar plasma was a gain medium of the Ar₂* excimer laser, which was produced by an intense femtosecond IR laser pulse. The VUV emissions from the plasma were confined by a couple of VUV optics that constructs an optical cavity. We have observed the amplification of the OFI Ar₂* excimer emission and evaluated the gain length product of 1.0 by using the optical cavity. The gain coefficient of 1.0 cm⁻¹ was evaluated by the gain-length value. We also observed the gain-length product of 5.0 by measuring the one-pass amplification inside a hollow fiber with the length of 5 cm, leading to the same gain coefficient. The function of the hollow fiber was, therefore, not for the OFI plasma regulation, but for the guiding of the VUV emissions as well as the IR femtosecond laser pulse.

5P108

VUV and X-ray metrological laboratory development on the base of the two storage rings. First experimental resultsS Anevsky¹, V Ivanov¹, P Kashkarov³, V Korchuganov³, M Kovalchuk³, V Krutikov², V Kvardakov³, V Lahov², A Lebedev³, O Minaeva¹, R Minaev¹, V Stankevich³, Y Zolotarevsky¹¹All-Russian Scientific Research Institute, Moscow, Russian Federation; ²Federal Agency on Technical Regulating and Metrology, Moscow, Russian Federation; ³Russian Research Center "Kurchatov institute", Moscow, Russian Federation

VUV and X-ray spectroradiometry is based on the use of synchrotron radiation of electron storage rings. VNIIOFI and RRC "Kurchatov institute" are developing common metrological laboratory on the base of the two storage rings SIBERIA-1 and SIBERIA-2. One of the main aims of the program is the progress in spectroradiometry based on the fundamental physical constants. We are going to use the reflecting telescope with VUV and X-ray CCD to recognize a single electron in the storage ring orbit. It will make possible to establish spectroradiometry units as spectral radiance, spectral radiant power e.t.c., based on single electron charge. Calibrations of CCD telescope with use of low-energy synchrotron radiation is based on absolute radiance spatial distribution. Experience of fruitful cooperation between VNIIOFI and PTB for 20 years, make possible to hope that metrological laboratory with the use of both storage rings will be successful. Electron storage rings SIBERIA-1 is kind of analogue of the MLS storage ring, thus particle energy can be change and let calibrate UV-VUV spectroradiometers with the use continuously adjustable beam current.

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XANES analysis techniques studying the phosphorus L-edges of soil organic matterC Ryan¹, L Zuin¹, C Scheffe², P Kappen³¹VLS-PGM Beamline, Canadian Light Source, Saskatoon, SK, Canada; ²Future Farming Systems Research Division, Department of Primary Industries, Rutherglen Center, Victoria, Australia; ³Centre for Materials and Surface Science and Department of Physics, La Trobe University, Victoria, Australia

Traditional standard X-ray absorption near-edge structure (XANES) spectroscopy analysis techniques prove to be either difficult or futile when analyzing data obtained in the vacuum ultraviolet (VUV) and soft X-ray energy ranges. With increasing attention being placed on the importance in characterizing the L_{2,3} edge spectra when determining third period elements (Al, P and S) speciation in complicated samples, a more defined analysis method should be discussed. Chemometrics is an evolving study using mathematical and statistical methods for handling, interpreting and predicting chemical data allowing for a more accurate characterization of unknown samples. Choosing the proper method of analysis is essential in assuring the accuracy of the result following the extraction of the factors from the spectral mixtures. Deconvolution, Linear Combination Fitting (LCF), Partial Least Squares (PLS), and Principal Component Analysis (PCA) will be considered. The advantages and disadvantages of choosing the correct technique will be investigated. Many techniques rely heavily on prior assumption of the spectral band and the initial guess supplied by the user. PCA will be the technique of primary interest as it does not have this dependency. PCA is a form of factor analysis; a multivariate technique for reducing matrices of data to their lowest dimensionality by the use of orthogonal factor space and transformations that yield predictions and/or recognizable factors (Malinowsky, 2002). These techniques were applied to an experiment measuring the phosphorus (P) L-edge XANES of soil organic matter to understand the chemical forms of P present, and to determine the impact of fertilizer and crop residue addition on P speciation. This experiment was conducted at 11ID-2, the Variable Line Spacing Plane Grating Monochromator (VLS-PGM) beamline at the Canadian Light Source (CLS). The results obtained will assist in determining the potential bioavailability of soil organic matter-bound P, simultaneously revealing the most effective tool for analysis.

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Pinching capillary discharge as a water window radiation sourceP Vrba,¹ SV Zakharov,² A Jancarek,³ M Vrbová,⁴ M Nevrkla,³ P Kolar⁴¹Institute of Plasma Physics, AS CR, Prague, Czech Republic; ²EPPRA sas, Villebon/Yvette, France; ³Czech Technical University in Prague, FNSPE, Prague, Czech Republic; ⁴Czech Technical University in Prague FBME, Kladno, Czech Republic

Our aim is to develop table-top monochromatic incoherent water window radiation source based on the pinching capillary discharge in nitrogen. We have performed preliminary experiments with alumina capillary (0.165 cm radius, 20 cm length), filled by nitrogen in the pressure range $20 \text{ Pa} < p_0 < 200 \text{ Pa}$. The discharge current with peak value $I_{\text{max}} = 13.5 \text{ kA}$ and quarter period $T_{1/4} = 75 \text{ ns}$ was achieved by discharging 13.5 nF capacitor through the capillary (initial voltage $U_0 = 70 \text{ kV}$). Strong spectral line at 2.88 nm, corresponding to the quantum transition $1s2p-1s^2$ of the helium-like nitrogen ions, was observed. Spatial and time evolutions of pinching plasma quantities as well as the water window emission were modeled by means of RHMD Z'-engine code. The dependencies of measured and evaluated water window output energy on the filling nitrogen pressure correspond each other for this experimental set up. For the optimum initial pressure the electron temperature $T_e \sim 30 \text{ eV}$ was evaluated in a wide volume of the discharge, remaining for a long time. Computer optimization of the device has been done by varying capillary geometry, charging voltage and initial pressure. It was forecasted that the output of water window radiation energy is decreasing with increasing capillary radius for given electrical circuit parameters. But, the dependence of pressure optimized output energy on the capillary length is not monotonous; the maximum of the output energy is expected when the capillary is 15 cm long. The experiments with the optimized capillary geometry are being prepared.

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5P111

Beamline for radiation source calibration in the VUV at the MLSR Thornagel,¹ R Fliegau,¹ R Klein,¹ W Paustian¹¹Physikalisch-Technische Bundesanstalt, Berlin, Germany

The Physikalisch-Technische Bundesanstalt (PTB), the German national metrology institute, performs synchrotron radiation based radiation source calibration in the VUV spectral range for about thirty years, traceable to the electron storage rings BESSY I and BESSY II. Since April 2008, PTB's own electron storage ring Metrology Light Source (MLS) [1] is in operation (see Poster R. Klein et al., this conference). A beamline for the calibration of radiation sources using the MLS as a primary radiation source is under construction and will be fully operational early 2011. The spectral range will cover the VUV region from 7 nm to 400 nm. It consists of a focusing elliptical mirror and a dedicated grating monochromator with a normal incidence and a grazing incidence configuration for the respective wavelength region. The whole mirror monochromator setup is built on a movable support frame so that it can be rotated around the incoming beam to account for the high degree of polarization of the synchrotron radiation. The monochromator can be flooded with gas between the entrance and the exit slits by means of integrated differential pumping stages acting as a gas filter with the objective of the reduction of higher order effects in the mid VUV spectral range.

[1] R. Klein et al., Phys. Rev. ST-AB 11, 110701 (2008).

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SOURCE, a VUV-UV synchrotron radiation beamline at the DAFNE-Light INFN-LNFE Pace,^{1,2} A De Sio,^{1,2} L Gambicorti,³ D Hampai,⁴ A Grilli,⁴ A Raco,⁴ G Viviani,⁴ M Pietropaoli⁴¹Dip. di Fisica e Astronomia, Università di Firenze, Firenze, Italy; ²INFN, Sezione di Firenze, Firenze, Italy; ³CNR-INO, Firenze, Italy;⁴INFN, Laboratori Nazionali di Frascati, Roma, Italy

DAΦNE-Light is the Synchrotron Radiation Facility at the INFN-Frascati National Laboratory (Rome, Italy). The synchrotron radiation (SR) photon beam from a wiggler installed on the DAΦNE storage ring is split by a grazing incidence Au-coated mirror ($\theta_i = 40 \text{ mrad}$, cut-off energy $\sim 800 \text{ eV}$), in order to provide the X-ray and UV beam lines. The reflected UV radiation travels through the UV beamline and ends in a three-channel experimental set up. The first light path is a near UV experimental apparatus, providing intense monochromatic irradiation ($\sim 10^{11} \text{ ph/s}$ on a $2 \times 7 \text{ mm}$ spot size) in the 200-450 nm spectral range. The second light path is the VUV channel operating in the 120-400 nm. The third channel is for wide-band UV irradiation. The beamline is partially operational since 2009 using the intense photon emission of DAΦNE, a 0.51 GeV storage ring with a routinely circulating electron current higher than 1 A, in *parasitic* and *dedicated mode*. This is operated for UV irradiation of biological materials, for astrobiology or astronomical applications, for material science, photo-biology, detector testing and development, for medical applications, for space instrumentation calibration and so on. This is especially devoted to experiments requiring very intense beams or for calibration of large space experiment.

5P113

Tunable high-harmonic source for time- and angle-resolved photoemission spectroscopy

G Dakovski,¹ Y Li,² T Durakiewicz,² G Rodriguez¹

¹Los Alamos National Laboratory, MPA-CINT, Los Alamos, NM, United States; ²Los Alamos National Laboratory, MPA-CMMS, Los Alamos, NM, United States

We present a laser-based apparatus suitable for visible pump/XUV probe time- and angle-resolved photoemission spectroscopy utilizing high-harmonic (HHG) generation from a noble gas. The laser system is a two-stage Ti:Sapphire multipass amplifier. The output is split in two arms, with approximately 90% of the energy being used for the process of HHG, and the remaining 10% used to optically excite the samples either at the fundamental or the second harmonic wavelengths. Using 1 mJ, 30 fs pulses at 800 nm, we obtain HHG up to 45 eV in a quasi-static gas cell filled with argon. Extraction of a single harmonic and tunability in a wide range of energies (currently 20–36 eV) is achieved by using a time-delay compensated monochromator (TDCM). The TDCM consists of two gratings in subtractive dispersion mode, operated in the off-plane mount, characterized by an excellent total throughput of ~10%. Using an amplified laser system at 10 kHz repetition rate, approximately $10^9 - 10^{10}$ photons/s per harmonic are made available for photoelectron spectroscopy. Parallel energy and momentum detection is carried out in a hemispherical electron analyzer (Phoibos 150) coupled with a two-dimensional imaging detector. First applications demonstrate the capabilities of the instrument to easily select the probe wavelength of choice, to obtain angle-resolved photoemission maps (GaAs), and to trace ultrafast electron dynamics in optically-excited (1.55 eV) semiconductor (Ge).

5P115

Development of LPP light source for extreme ultraviolet microscope

T Ejima,¹ S Aizawa,¹ M Furudate,¹ T Hatano,¹ M Yanagihara¹

¹IMRAM, Tohoku University, Sendai, Japan

Laser produced plasma (LPP) light source is known as one of EUV ones, and EUV light emitted from this light source is generated by plasma, which is produced when an excitation laser light irradiates a metallic target. Because duration time of LPP light source is comparable to that of the excitation laser, microscopic observation with short exposure time will be possible by the use of this light source. Minute structures of "active" living organisms move by the Brownian motion, for example, a $1 \mu\text{m}$ cell in diameter will move 20 nm in 1 msec at RT [1]. Therefore, reducing the exposure time less than 1 msec is necessary to observe a 20 nm structure within a $1 \mu\text{m}$ cell. The duration time of pulsed Nd:YAG lasers is tens of nsec for 1 shot of a laser pulse, and about 2 orders shorter than the exposure time for 20 nm structure observation. On the other hand, the plasma emits debris, which pollutes the optical system and decreases EUV throughput of the microscope. Therefore, decreasing debris is preferable for the performance of the microscope. In this study, we investigated target materials and angle dependence of both EUV emission intensity and the amount of the debris for quality and stability of our developing EUV microscope [2]. Measurement result suggests that the pollution of the optics will be decreased by a layout of both target and optics, because the angle distribution of EUV emission was isotropic but that of debris, anisotropic in W plane target. [1] A. Ito and K. Shinohara, Cell Struct. Func., 17, 209-212 [1992]. [2] T. Ejima, et al., Opt. Express 18, 7203-7209 [2010].

5P116

Pre-plasma dependence of relativistic surface harmonic generation

M Behmke,¹ C Rödel,³ DAD Brügge,² M Heyer,³ O Jäckel,³ D Hemmers,¹ T Toncian,¹ A Pukhov,² O Willi,¹ GG Paulus,³ G Pretzler¹

¹Institut für Laser und Plasmaphysik, Heinrich-Heine-Universität, Düsseldorf, Germany; ²Institut für Theoretische Physik I, Heinrich-Heine-Universität, Düsseldorf, Germany;

³Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität, Jena, Germany

We report on experimental investigations about the influence of pre-plasma conditions onto the generation of relativistic surface harmonics. These experiments have been performed using a 100 TW Ti:Sa laser (ARCTURUS, Düsseldorf University) with a pulse duration of 28 fs and intensities of about 10^{12} W/cm² in the focus. In order to change the pre-plasma formation we modified the contrast of the laser pulse by varying the target-surface of a plasma mirror. Depending on the contrast the recorded spectra show significant differences in shape and envelope. We provide a semi-analytical model to explain the recorded spectra, which is backed up by PIC simulations showing analogous results. The combination of different approaches allows a deeper understanding of the processes at the vacuum-plasma interface during the relativistic surface harmonic generation.

5P117

Future plan of the HiSOR lightsource

A Miyamoto,¹ K Goto,¹ S Hanada,² S Sasaki,¹ H Namatame,¹ M Taniguchi¹

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan

The HiSOR is a compact synchrotron light source of Hiroshima Synchrotron Radiation Center constructed in 1996 as a VUV ~ soft X-ray source. Due to the nature of compact racetrack-type storage ring, its natural emittance is as large as 400 nm-rad which is not so small as those of other larger rings. There are two undulators installed in the straight sections, one linear for 26-300 eV range and the other helical/linear for 4-40 eV. The most outstanding feature of the facility lies in the good combination among the light sources, beamlines, and experimental stations to attain ultra high resolution for the photoelectron spectroscopy. The HiSOR has been running over the decade, thus, it is the time to consider possible future improvements of the facility. The motivation is to pursue the leading position in the field of solid state physics and materials/nano science including photoelectron spectroscopy and spin resolved photoemission spectroscopy by using VUV radiation. Therefore, the construction of the low emittance compact VUV lightsource ring, HiSOR-II, is planned. In this paper, we present the current status of HiSOR, a design feature of HiSOR-II, and expected performance.

5P118

Quasi-periodic variable polarization undulator for HiSORS Sasaki,¹ A Miyamoto,¹ K Goto,¹ H Namatame,¹ M Taniguchi¹¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan

The Hiroshima Synchrotron Radiation Center of Hiroshima University is a unique VUV light source facility. It is equipped with a small racetrack type storage ring nicknamed HiSOR. This ring has the electron beam energy of 0.7 GeV, the maximum beam current of 350 mA, and the beam emittance of 400 nm-rad. In this ring, two undulators, a 100-mm-period elliptical undulator and a 57-mm-period linear undulator, are installed in order to serve high-flux photon beams with energy ranges in UV-VUV for multiple user experiments. Recently, these undulator beamlines are oversubscribed mainly for the high precision photo-electron spectroscopy experiments to investigate electronic properties of newly found exotic materials including the Fe-based high-Tc superconductors. For this reason, we decided to construct a new undulator to meet users' requirements. The new device will be an APPLE-II type variable polarization undulator with an option of quasi-periodicity [1,2]. The design feature was selected so that the new undulator generates higher flux than that by a current helical undulator. This new undulator has the 78-mm period length and the number of period of 24. The lowest achievable photon energy should be 6 eV for any polarization mode including the vertical linear polarization. To meet this users' requirement, the undulator parameter, K , needs to be as large as 4.2. For such a large K -value, the contamination from higher harmonics in the flux spectrum is not negligible even in the circular mode. Therefore, the quasi-periodic option is considered [3]. In this paper, a detailed design feature and expected performance are presented.

[1] S. Sasaki, Nucl. Instrum. Methods A 347 (1994) 83.

[2] S. Sasaki, B. Diviacco, R.P. Walker, Proceedings of 1998 European Particle Accelerator Conference, p.2237.

[3] B. Diviacco, et al, Proceedings of 2000 European Particle Accelerator Conference, p.2322.

5P119

Interference effects in two-color high-order harmonic generationR Rakowski,¹ X He,¹ JM Dahlström,¹ C Heyl,¹ A Persson,¹ J Mauritsson,¹ A L'Huillier¹¹Department of Physics, Lund University, Lund, Sweden

We have investigated experimentally and theoretically high-order harmonic generation in Ar gas cell with a bichromatic 800/400 nm intense laser field. The use of two-colors, an infrared fundamental beam of a Ti:sapphire system (40 TW, 10 Hz, 40 fs) and its second harmonic makes it possible to subcycle control the driving electric field. Even and odd harmonics are generated, with intensity and divergence strongly modulated as a function of the relative time delay between the two color fields. We show how these oscillations depend on harmonic energy, intensity of the blue field and how the spatial profiles are affected. We present an analysis of the interference effects responsible for the results. A blue field allows us to characterize the resulting attosecond pulses, which have an average duration of 380 as and a few tens of nJ energy. We also discuss a switch of the dominant trajectory responsible for harmonic generation when approaching the cutoff region.

5P120

Picosecond precision time-of-flight photoelectron measurementsP Hammond,¹ AJ Alderman,¹ BG Birdsey,¹ TJ Reddish,² A Padmanabhan,² PA Thorn,^{1,2} KC Prince,³ R Richter,³ V Feyer³¹School of Physics, CAMSP, University of Western Australia, Perth, Western Australia, Australia; ²Department of Physics, University of Windsor, Windsor, Ontario, Canada;³Sincrotrone Trieste, Basovizza, Trieste, Italy

We have invented and developed a new ultrafast photoelectron timing system called a Delayed Electron Emission Detector (DEED) capable of making picosecond precision time-of-flight measurements. DEED has been tested and developed using XUV light (<100eV) on the Gas Phase Beamline at Sincrotrone Trieste. DEED incorporates an internal delay unit externally variable with picosecond precision with respect to the synchrotron orbit clock to which DEED is synchronised. The aim is to allow the detection of photoelectrons emitted from autoionising states time delayed after the exciting photon pulse and hence be a complimentary technique to delayed fluorescence experiments [1]. The system is also likely to be very appropriate for use with Free Electron Laser light sources and find application to time of flight studies of photoions. Diagnostic measurements of the multibunch photon light pulses spaced by 2 ns and of temporal width ~80 ps can be achieved with a timing resolution of < 40 ps over a linear timing window of width 6 ns – which itself can be extended to hundred's of nanoseconds giving a broad dynamic range for the system. The timing resolution of DEED is considerably better than the temporal width of the light pulses currently available at Elettra and further optimisation of the system therefore requires access to shorter light pulses.

[1] Lambourne *et al*, Phys.Rev.Lett. (2003) **90**, 153004

5P121

Pinching capillary discharge as a source of radiation below 50nmM Nevrkla,¹ A Jancarek,¹ P Vrba,² M Vrbova³¹Czech Technical University, Prague, Czech Republic; ²Institute of Plasma Physics, ASCR, Prague, Czech Republic; ³Czech Technical University, Kladno, Czech Republic

Our aim is to develop table-top monochromatic incoherent water window radiation source based on the pinching capillary discharge in gas. We have performed several preparatory experiments with alumina capillary (0.165 cm radius, 21 cm length), filled by Argon in the pressure range $5 \text{ Pa} < p_0 < 1000 \text{ Pa}$. The discharge current with peak value $I_{\text{max}} = 11 \text{ kA}$ and quarter period $T_{1/4} = 75 \text{ ns}$ was achieved by discharging 15 nF capacitor, initially charged to $U_0 = 80 \text{ kV}$. Strong spectral line at 46.9 nm, corresponding to the quantum transition $3s^1p_1 \rightarrow 3p^1S_0$ of the Neon-like Argon ions, was observed by XRD at pressure 13 Pa. This XUV signal was observed at 40 ns practically in time of pinch [1]. The experiments with higher value, 65 Pa of Argon pressure, led to observation of the spike XRD signal in second quarter of current pulse. XUV signal was observed cca 20 ns after pinch. This signal probably corresponds to recombination pumping. Our preliminary calculations prompt that it could be radiation of Beryllium-like Argon with 42.6 nm wavelength [2].

[1] A. Jancarek et al., Proceedings of 29th ICPIG, Cancun, Mexico [2009][2] Yasushi Hayashi et al., Jpn. J. Appl. Phys. **42** [2003] pp. 5285-89

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5P122

New operation modes of electromagnetic EPUS Qiao¹¹Fudan University, Shanghai, China

Heat load on beamline optics is a serious obstacle for devices designed to generate pure linearly polarized photons in third generation synchrotron radiation facilities. For permanent magnet undulators, this problem can be overcome by implementing a figure-eight design configuration. As yet there has been no good method to tackle this problem for electromagnetic EPU (elliptical undulators). Here, some new operation modes [1,2] of electromagnetic EPU are suggested, which can generate pure linearly polarized photons at an arbitrary polarization direction with very low on-axis heat load. Additionally, the minimum photon energy capability of linearly polarized photons can be significantly extended. The switching between normal EPU (for circular polarized photon) and knot, leaf modes (for linear polarized photon) can be achieved by only a switch box to connect the magnets with different diagrams, which makes the switching very practicable.

[1] S. Qiao, Dewei Ma, Donglai Feng, S. Marks, R. Schlueter, S. Prestemon, and Z. Hussain, Knot undulator to generate linearly polarized photons with low on-axis power density, Rev. Sci. Instrum. **80**, 085108 [2009].

[2] J. Yan, S. Qiao, Leaf undulator to realize polarization control with low on-axis heat load, to be published in Rev. Sci. Instrum.

5P123

Sulfur speciation of long-term fertilized soils assessed by XANESL Liu,¹ M Cui¹¹Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China

X-ray absorption near edge structure (XANES) of sulfur K-edge was used to determine the proportion of S at different oxidation states and assess the impact of different long-term fertilization on the form, amount of S in different type soil. Soil samples were collected at different areas in China. XANES spectroscopy showed that all of most reduced S (sulfides, disulfide, thiols, and thiophenes), highly oxidized S (ester-SO₄²⁻, and sulfate) and intermediate S (sulfoxides and sulfonates) are present in all different soil, the rates of different oxidized S are different, and that the most proportion is highly oxidized S and intermediate S is the least. Long-term fertilization had a profound influence on the relative proportion of different oxidized S in soil. Different fertilizer made the proportion of different oxidized S in soil change.

5P124

Characterization of impregnated NaY Zeolites by X-ray absorption and emission spectroscopies

A Guerra,¹ G Ferreira,² C Turci,² M Franco,² N Rosenbach Jr.,² B Kover,² C Mota²

¹DEPBG-CEFET/RJ, Rio de Janeiro/RJ, Brazil; ²Instituto de Química-UFRJ, Rio de Janeiro/RJ, Brazil

The carbocation γ reactions by nucleophilic substitution have been studied using halogenated NaY zeolites as a solid solvent. A better comprehension of the rearrangements and nucleophilic substitutions and halogens exchanges in the inner zeolites structures leads to the development of more powerful manufacturing catalysts. Our goal is to characterize various impregnated halogens NaY zeolites and to study the ionization potential (IP) and the electronic transitions of these samples by X-ray absorption and emission spectroscopies, using synchrotron radiation. *Ab initio* calculations associated with Gamess, GSCF3 and IVO methods have been used to optimize part of the geometries and to help us in the assignments. The experiments were performed using the Soft X-ray Spectroscopy (SXS) beamline at the National Laboratory of Synchrotron Light (LNLS) in Campinas-SP, Brazil. The samples were prepared by impregnation over commercial NaY zeolite using NaF, NaCl, NaBr and NaI aqueous solutions and dehydrated at 400°C. They were introduced into the main chamber as a solid supported by a carbon sticky tape. The work pressure was maintained at 2×10^{-8} mBar. The X-ray absorption near edge spectra (XANES) of the zeolites have been measured at Si 1s and Cl 1s edges and the X-ray photoelectron spectra (XPS) at O 1s, Na 1s, Al 1s, Si 1s, F 1s, Cl 1s, Cl 2p, Br 2p_{1/2} and I 3d_{5/2} edges. Long scan XPS spectra were obtained to help the assignments (LNLS - proposal D08A-SGM-7730).

5P125

Electronic properties of the neutral coordination compounds of the DMIT ligand in the S 1s region

LJS Lopes,¹ NM Comerlato,¹ GB Ferreira,¹ ACO Guerra,² CC Turci¹

¹Instituto de Química – UFRJ, Rio de Janeiro/RJ, Brazil; ²CEFET-RJ, Rio de Janeiro/RJ, Brazil

Polisulphurated ligands represent a very important class of coordination compounds, due to your several applications as charger transfer salts on the development of high technology electronic materials. The 1,3-dithiole-2-thione-4,5-dithiolate ligand (DMIT) represents one of the main polysulfur systems of this class. Our goal is to characterize various coordination compounds of DMIT ligand with different transition metals. Photoabsorption and Photoelectron S1s spectra of DMIT complexes have been acquired for [Ni(Dmit)₂][NEt₄]₂, [Cu(Dmit)₂][NEt₄]₂, [Zn(Dmit)₂][NEt₄]₂ and [Co(Dmit)₂][NEt₄]₂. All compounds were synthesized following the literature. TEY and XPS spectra have been acquired at Soft X-ray Spectroscopy (SXS) beamline, at LNLS-Campinas-SP, Brazil. The samples were introduced into the main chamber as a solid using a carbon sticky tape. The work pressure was kept at $\sim 2 \times 10^{-8}$ mBar. The ionization potentials (IP) of these compounds have been determined and the electronic transitions have been studied. *Ab initio* calculations, associated with improved virtual orbital (IVO) method, carried out using the GSCF3 program, were considered to help us with the assignments. The geometric parameters were optimized with the GAMESS program. The differences observed in the TEY spectra may be related to the different structures of the compounds.

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5P126

Soft X-ray absorption and photoemission spectroscopy study of superoxide KO₂

BI Min,¹ M Kim,¹ HL Park,¹ YH Jeong,¹ JY Baik,² HJ Shin,² DH Kim,³ JH Hwang,³ JS Kang³

¹Physics, POSTECH, Pohang, Republic of Korea; ²Pohang Accelerator Laboratory, POSTECH, Pohang, Republic of Korea; ³Physics, The Catholic University of Korea, Bucheon, Republic of Korea

In alkali superoxides AO₂ (A= Na, K, Rb), the partially occupied anti-bonding π^* molecular states of the localized O 2p orbitals are considered to play an important role in determining their electronic and magnetic properties. We have studied the electronic structure of KO₂ by employing soft X-ray absorption spectroscopy (XAS) and core-level photoemission spectroscopy (PES). We have also compared the measured O 1s XAS spectrum with the calculated partial density of states (PDOS), which was obtained from the first principles electronic structure calculations by including the spin-orbit effect and the on-site Coulomb interaction between O 2p electrons. K 2p and O 1s core-level PES spectra confirm the good quality of the KO₂ sample, employed in this study. It is found that the unoccupied states, which are determined from the measured O 1s XAS, agree reasonably well with the calculated PDOS's, suggesting the importance of the spin-orbit effect and the on-site Coulomb interaction between O 2p electrons in KO₂.

5P127

Structural properties of low-temperature grown ZnO thin films determined by X-ray diffraction and X-ray absorption spectroscopy

IJ Lee,¹ CJ Yu,¹ NE Sung,¹ YD Yun,¹ HK Lee,¹ HJ Shin¹

¹Beamline Division, PAL, POSTECH, Pohang, Republic of Korea

The epitaxial growth of ZnO thin films on Al₂O₃ (0001) substrates have been achieved at a low-substrate temperature of 150°C using a dc reactive sputtering technique. The structures and crystallographic orientations of zinc oxide films varying thicknesses on sapphire (0001) were investigated using X-ray diffraction (XRD), angle-dependent X-ray absorption near-edge structure (XANES), and extended X-ray absorption fine structure (EXAFS) spectroscopy with linearly polarized X-rays. The XRD data showed that the crystallinity of the film is improved as the film thickness increases and the strain is fully released as the film thickness reached about 800 Å. The Zn K-edge XANES spectra of the ZnO films have a strong angle-dependent spectral feature resulting from the preferred *c*-axis orientation. All the results consistently suggest that dc sputtered ZnO films are wurtzite structure with the preferred *c*-axis orientation.

5P128

Investigation of coordination changes in substituted transition-metal oxides by K-edge XANES: beyond the pre-edge

AP Grosvenor,¹ MW Gaultois¹

¹Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada

Transition-metal oxides are important materials having many applications, including; catalysis, semi-conductor devices, ion-conductors, and as multiferroic materials. The properties of these materials can be tuned through selective substitution of the constituent elements. For oxygen deficient materials, substitution of one metal for another, having a different oxidation state, can lead to variations in coordination number (CN). Studies of first-row transition-metal K-edge XANES spectra can lead to information on changes in CN through examination of the pre-edge peak intensity, resulting primarily from a 1s to *n*-1d transition. However, investigation of pre-edge peaks from second-row transition-metals can be difficult owing to lower spectral resolutions at higher excitation energies. Noting this, it has been observed that changes in CN lead to significant variations in intensity and energy of the main absorption edge (1s to *np* transition), an observation which is rarely reported. Examination of all three spectral changes, by analysis of a 3D plot, can be used to accurately investigate changes in CN with substitution. During this presentation, the study of K-edge spectra from substituted first and second-row transition-metal oxides and silicates will be described. The systems that will be reported on include substituted Brownmillerite-phase oxides (e.g., Ca₂Fe_{2-2x}Ga_xO₅), oxygen deficient perovskites (e.g., SrFe_{1-x}Zr_xO_{3-δ}), and amorphous transition-metal silicates (e.g., (ZrO₂)_x(SiO₂)_{1-x}).

5P129

Role of oxygenation on the reactivity of Ru-S bonds in arene anticancer agents: Insights from XAS and DFT

T Sriskandakumar,¹ H Petzold,² PCA Bruijninx,³ A Habtemariam,³ PJ Sadler,³ P Kennepohl¹

¹Department of Chemistry, University of British Columbia, Vancouver, BC, Canada; ²School of Chemistry, University of Edinburgh, Edinburgh, United Kingdom; ³Department of Chemistry, University of Warwick, Coventry, United Kingdom

We have investigated thiolato ligand oxygenation in a series of organometallic half-sandwich Ru arene [(η⁶-arene)Ru(*en*)(SR)]⁺ anticancer agents. X-ray Absorption Spectroscopy, in concert with density functional theory calculations, has been used to describe the influence of thiolato oxygenation on the nature of Ru-S bond including the effect on arene and thiolato ligand modifications in the parent thiolato and mono- and di-oxygenated sulfenato and sulfinato species respectively. Data showed that Ru_{4d} ← S_{3p} charge donation changes as a function of oxidation state of the sulfur atom, but that has little impact on overall ligand charge donation to the metal center due to varying contributions from the terminal oxo group. Small electronic modifications in the thiolato complexes are amplified in the oxidized species, which has direct implications in optimizing the design of these complexes. Our studies suggest that the sulfenato species are most susceptible to ligand exchange via activation by as protonation of the terminal oxo group. Further investigation of sulfenato activation is going on.

5P130

The electronic structure of azafullerene encapsulated single-walled carbon nanotubes

H Yagi,¹ Y Tokumoto,¹ Y Aoki,¹ M Zenki,¹ T Zaima,¹ T Miyazaki,¹ S Hino,¹ N Tagmatarchis,² Y Iizumi,³ T Okazaki^{3,4}

¹Graduate School of Science and Engineering, Ehime University, Matsuyama, Japan; ²Theoretical and Physical Chemistry Institute, Athens, Greece; ³Nanotube Research Center, AIST, Tsukuba, Japan; ⁴PRESTO, JST, Kawaguchi, Japan

Single walled carbon nanotubes (SWCNTs) encapsulating fullerenes, so called fullerene peapods, have attracted considerable interests as candidates for the new nano-electronic materials. C₅₉N@SWCNT is the first fullerene peapods that exhibits n-type FET characteristics while pristine SWCNT FET and C₆₀@SWCNT FET are p-type. We measured ultraviolet photoelectron spectra (UPS) of C₅₉N@SWCNT and SWCNT to investigate how the electronic structure is modified by the encapsulation of C₅₉N. The work function of C₅₉N@SWCNT, which can be estimated from the secondary electron cutoff of UPS, is almost the same as that of SWCNT. Some additional peaks are observed in the UPS of C₅₉N@SWCNT compared with that of SWCNT. The spectrum of encapsulated C₅₉N pea is obtained by subtracting the spectrum of SWCNT from that of C₅₉N@SWCNT. The spectrum of C₅₉N pea is analogous to that of [C₅₉N]₂ thin film, which might indicate that most of C₅₉N molecules are entrapped in the SWCNTs in a form of dimer. It should be noted that the C₅₉N pea spectrum shifted by about 0.1 eV toward lower binding energy and the HOMO -2 peak became slightly narrower than that of [C₅₉N]₂.

5P131

Simultaneous detection of X-ray fluorescence and conversion electrons for site specific XAFS characterization of supported Rh catalysts

S Hayakawa,¹ H Koga,¹ H Sumida,² Y Oumi,¹ T Sano,¹ H Namatame,³ T Hirokawa¹

¹Department of Applied Chemistry, Hiroshima Univ., Hiroshima, Japan; ²Technical Research Center, Mazda Motor Co, Hiroshima, Japan; ³Hiroshima Synchrotron Radiation Center, Hiroshima Univ., Hiroshima, Japan

X-ray absorption fine structure (XAFS) measurements are widely utilized for characterization of automotive exhaust catalysis because XAFS provides local structural and chemical information of element of interest. By utilizing difference of probing depths between X-ray fluorescence yield (XFY) and conversion electron yield (CEY), chemical states of Rh/γ-Al₂O₃ catalyst were discussed with the site selective XAFS spectra. Two types of Rh/γ-Al₂O₃ samples were prepared by sol-gel process and by impregnation process. Samples were characterized with X-ray diffraction and transmission electron microscope (TEM). XAFS experiments were performed on the BL-11 of HiSOR by using a He filled chamber equipped with an electrode for collecting conversion electrons, and both XFY and CEY were measured simultaneously [1]. The magnitude of the white line of the obtained Rh L₃-edge XAFS spectra indicated relative measure of the oxidation state. The Rh sample prepared by the sol-gel process showed slightly larger white line compared to that prepared by the impregnation process when measured with the CEY method. The greater white line was obtained with the same impregnated sample by the XFY method. The results indicated that Rh supported onto the inner surface of γ-Al₂O₃ was in the higher oxidation state compared to that was mainly investigated with the CEY method.

[1] S. Hayakawa et al., Anal. Sci. 24, 835(2008).

5P132

Shifts in SrFe_{1-x}Zn_xO_{3-δ} absorption energies and binding energies: influencing the magnitude of final-state relaxation by changing the metal coordination number

MW Gaultois,¹ AP Grosvenor¹

¹Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada

Perovskite-type mixed ionic-electronic conduction (MIEC) oxides have received considerable attention as catalytically-active electrodes, solid electrolytes, and oxygen separation membranes. These materials have the general formula ABO_{3-δ} (A = alkaline-earth; B = transition-metal); partial substitution of metal cations leads to an oxide anion deficiency, which, due to ordering of these vacancies, can lead to ionic conductivity. Owing to their lack of chemical durability, alternatives to Co-based MIEC materials are being investigated, with systems similar to SrFe_{1-x}Zn_xO_{3-δ} having been proposed as new high oxygen-flux ceramics. In this work, the SrFe_{1-x}Zn_xO_{3-δ} system (0 ≤ x ≤ 1) was synthesized and investigated by X-ray absorption near-edge spectroscopy (XANES) and X-ray photoelectron spectroscopy (XPS). These techniques were used to examine the effect of substitution on metal charge and coordination number, and to study the influence of ground-state and final-state effects on spectral energies. Substitution of Zn for Fe results in shifts in XPS binding energies (Sr 3d, Zn 2p, Fe 2p, and O 1s) and K-edge XANES absorption energies (Zn and Fe) that are much greater than the shifts observed in the Fe L- and Zn L-edge XANES absorption energies. This presentation will expose the cause of these shifts; a change in coordination number alters the magnitude of final-state relaxation, which depends on the principal quantum number and angular momentum of the electron excited. The importance of this work to developing a better understanding of the influence of final-state next-nearest-neighbour effects on binding and absorption energies will also be presented.

5P134

Photoemission spectroscopy of AT_4Sb_{12} (A=Ca, Sr, Ba; T=Fe, Ru)

H Sato,¹ M Higashi,² K Yoshikawa,² E Matsuoka,³ K Hayashi,⁴ S Narazu,⁴ T Takabatake,⁴ M Nakatake,¹ H Namatame,¹ M Taniguchi^{1,2}

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan;

³Graduate School of Science, Kobe University, Kobe, Japan; ⁴ADSM, Hiroshima University, Higashi-Hiroshima, Japan

Filled-skutterudite compounds have attracted a great interest because of the thermoelectric application as well as unusual physical properties. In comparison with rare-earth filled compounds, alkaline-earth filled ones have less been studied. Recently, Takabatake *et al.* have prepared AT_4Sb_{12} (A=Ca, Sr, Ba; T=Fe, Ru, Os) polycrystals and reported their magnetic and transport properties [1]. In this study, we have investigated electronic structure of AT_4Sb_{12} (A=Ca, Sr, Ba; T=Fe, Ru) by means of photoemission spectroscopy (PES) at BL7 of HiSOR. From the valence-band PES spectra, we find that the center of gravities of the T d bands shift toward deeper binding energy side as going from T=Fe to Ru and the features of the Fe 3d and Ru 4d density of states (DOS) are almost independent of A-elements. The Fe 3d DOS largely contributes to the Fermi level (E_F), while few Ru 4d DOS is observed at E_F . These experimental results are qualitatively consistent with the results of almost A-independent electric specific coefficients; ~ 100 (AFe₄Sb₁₂) and 10 mJ/mol K² (ARu₄Sb₁₂) [1]. The Fe 3d DOS and the energy shift of the d bands are well explained by the band-structure calculations, while the Ru 4d DOS locates in the deeper binding energy region slightly than that of the calculations [2].

[1] T. Takabatake *et al.*, Physica B **383**, 93 [2006].

[2] K. Takegahara *et al.*, J. Phys. Soc. Jpn. **77**, 294 [2008].

5P135

Complementary studies of structural characteristics and properties for smooth redeposited hydrocarbon films from T-10 tokamak with synchrotron radiation and neutrons

VG Stankevich,¹ YV Zubavichus,¹ AA Veligzhanin,¹ VA Somenkov,¹ NY Svechnikov,¹ KA Menshikov,¹ AM Lebedev,¹ LN Khimchenko¹

¹Russian Research Center Kurchatov Institute, Moscow, Russian Federation

Smooth homogenous hydrocarbon films, or "flakes" [with atomic ratio D/C $\approx 0.5-0.8$, H/C ~ 0.2 , thickness $\sim 30 \mu\text{m}$], redeposited under fluctuations of the edge plasma in tokamaks onto the vessel wall regions far from graphite plasma facing components, may accumulate much protium, deuterium and tritium [1, 2]. The properties of such films, formed from T-10 tokamak deuterium plasma discharge, are reported from SAXS, WAXS measurements for X-rays and neutrons, VUV-VIS photoluminescence, NEXAFS and EPR. The overall structural pattern resembles the pattern for an amorphous solid, with graphene-like sheets composed from aromatic rings oriented mainly parallel to the film surface. This structure is strongly disturbed by broken bonds and a presence of a high density micropores filled with deuterium. The latter results in the first large X-ray diffraction peak, not observable for neutrons due to comparable carbon-deuterium contrast, while the other two graphene-like peaks are similar for X-ray and neutron observations. The material displays the mixed sp²-sp³ properties of a wide-band semiconductor with a gap of about 3 eV. The EPR observable defects with unpaired spins refer to broken π -bonds in Csp²- nano-clusters which size is ~ 4 nm and spin orientation is non-isotropic.

[1] N.Yu. Svechnikov, V.G. Stankevich, et al. J. Surf. Invest., **3** (3) 420 [2009].

[2] N.Yu. Svechnikov, V.G. Stankevich, et al. Plasma Dev. Oper. **14** (2), 137 [2006].

5P136

Itinerant spin fluctuations and electronic structure in $CeFeAsO_{1-x}F_x$ iron-oxypnictides

F Bondino,¹ E Magnano,¹ F Offi,² G Panaccione,¹ M Malvestuto,³ G Paolicelli,⁴ L Simonelli,⁵ F Parmigiani,⁶ MA McGuire,⁷ AS Sefat,⁷ BC Sales,⁷ R Jin,⁸ D Mandrus,⁷ DJ Singh,⁷ N Mannella⁸

¹IOM CNR, Laboratorio TASC, Basovizza, Trieste, Italy; ²CNISM and Dipartimento di Fisica, Università Roma Tre, Roma, Italy; ³Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy;

⁴CNR-INFM, National Research Center S3, Modena, Italy; ⁵European Synchrotron Radiation Facility, Grenoble, France; ⁶Dipartimento di Fisica, Università degli Studi di Trieste, Italy;

⁷Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, United States; ⁸Physics Department, University of Tennessee, Knoxville, TN, United States

The new class of high-temperature superconductors (HTSs) in layered iron arsenic compounds [Y. Kamihara, et al., J. Am. Chem. Soc. **130**, 3296 [2008]] has generated enormous interest. Important challenges are to understand the interplay between the fluctuations associated with the apparent proximity to magnetism and the superconducting phase and the differences/similarities between these materials and the cuprate HTSs. We have performed an extensive study on the intrinsic bulk electronic structure of the HTS $CeFeAsO_{0.89}F_{0.11}$ and its parent compound $CeFeAsO$ by soft and hard X-ray photoemission, X-ray absorption and soft-x-ray emission spectroscopies. The complementary surface/bulk probing depth, and the elemental and chemical sensitivity of these techniques allows resolving the intrinsic electronic structure of each element. The data reveal signatures of Fe d-electron itinerancy, which suggests that the underlying physics and the origin of superconductivity in these materials are likely to be quite different from those of the cuprate HTSs. Furthermore, our experiment provides a strong and unique test case for occurring of itinerant magnetic fluctuations, whose detection has been made possible by the extremely fast time scales proper of the photoemission process [F. Bondino et al. Phys. Rev. Lett. **101** (2008) 267001].

5P137

Photoemission spectra of frozen rock salt $\text{Pb}_{1-x}\text{Cd}_x\text{Te}$ crystal

BA Orłowski,¹ A Szczerbakow,¹ BJ Kowalski,¹ MA Pietrzyk,¹ K Gas,¹ M Szot,¹ W Szuszkiewicz,¹ V Domukhovski,¹ S Mickevicius,² RL Johnson,³ S Thiess,³ W Drube³

¹Institute of Physics PAS, Warsaw, Poland; ²Semiconductor Physics Institute, Vilnius, Lithuania; ³HASYLAB am DESY, Hamburg, Germany

The nanostructures with a quantum dots of PbTe (rock salt, band gap 0.23eV) in CdTe (zinc blende, band gap 1.45eV) and CdTe dots in PbTe are of great interest of application as well in thermoelectric devices as in infrared detectors. The bulk single crystals of $\text{Pb}_{1-x}\text{Cd}_x\text{Te}$, were grown by physical vapour transport (PVT) method and with proper quenching [1]. The frozen rock salt crystals of $\text{Pb}_{1-x}\text{Cd}_x\text{Te}$ ($x=0.06, 0.08, 0.15$) about 1cm with (001) oriented natural facets were obtained. Photoemission Spectroscopy (Tunable High Energy PES and Ultraviolet PES) were applied to study the crystals spectra containing: valence band, Cd3d and 4d, Pb 4f and 5d and Te 3d and 4d. The experiment was performed using the THE-XPS spectrometer at wiggler beam line station BW2 of the HASYLAB, DESY, Hamburg, Doris III storage Ring. The station E1 with the FLIPPER II monochromator was used to obtain ultraviolet PES spectra. The chemical shift of the core levels and the appearance of shoulders of the core peaks were studied to illustrate the interaction with different nearest neighbors. The valence band density of states distribution spectra remarkably changes with the crystal composition. X-ray diffraction studies recognized kind of defects suggesting the preference to create the dots of PbTe while the other defects can be correlated to the preference of CdTe dots creation. The results will be discussed with the theoretical calculation of competition minimum of energy for creation CdTe or PbTe dots.

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1. M. Szot, at all, Acta Phys. Pol. 116, 959 (2009).

5P138

GeTe and $\text{Ge}_{0.9}\text{Mn}_{0.1}\text{Te}$ valence band structure – an angle-resolved photoemission study

BJ Kowalski,¹ MA Pietrzyk,¹ R Nietubyc,² W Knoff,¹ BA Orłowski,¹ A Lusakowski,¹ J Sadowski,^{1,3} T Story¹

¹Institute of Physics, Polish Academy of Sciences, Warsaw, Poland; ²The Andrzej Soltan Institute for Nuclear Studies, Swierk/Otwock, Poland;

³MAX-lab, Lund University, Lund, Sweden

The valence band structure have been determined for GeTe and $\text{Ge}_{0.9}\text{Mn}_{0.1}\text{Te}$ along the Γ -T and T-W-L directions in the Brillouin zone by angle-resolved photoelectron spectroscopy. The study was motivated by the need for deepening the knowledge of properties of $\text{Ge}_{1-x}\text{Mn}_x\text{Te}$ - a semiconducting system exhibiting ferromagnetism up to the relatively high temperature of 190 K and considered as a material suitable for future spintronic applications. The GeTe and $\text{Ge}_{0.9}\text{Mn}_{0.1}\text{Te}$ epilayers were grown along the [111] direction by MBE on BaF_2 substrates. The sets of photoemission spectra were taken with use of synchrotron radiation in MAXlab synchrotron radiation laboratory of Lund University (Sweden). The experimental band structure diagrams $E(k)$ were derived from the acquired data with use of the free-electron final state model. These experimental results were compared with the electronic structure of GeTe obtained by *ab initio* fully relativistic LDA pseudopotential calculations. The features that can be ascribed to emission from Mn states were revealed, mainly 3.5 eV below the valence band edge. The main parameters describing the rhombohedral primitive cell of the system were also derived from this comparison.

5P139

Phase composition and oxidation states of gas-sensitive materials: analysis by X-ray absorption spectroscopy and photoelectron spectroscopy

GE Yalovega,¹ VA Shmatko,¹ TN Nazarova,² OV Zabluda,² VV Petrov,² GY Smolentsev^{1,3}

¹Department of Physics, Southern Federal University, Rostov-on-Don, Russian Federation; ²Taganrog Institute of Technology, Southern Federal University, Rostov-on-Don, Russian Federation; ³Department of Chemical Physics, Lund University, Lund, Sweden

Due to increasing requirements to the sensors characteristics the high priority has been given to the materials containing metals oxides, in particular to copper oxides or mixture of them with other oxides. They show gas sensitivity to different pollutants and can be applied as sensors for quality air control. The stored solutions were exposed to temperature treatment of 150, 300, 500 and 700°C. To investigate the phase composition and oxidation states of the novel materials the methods of X-ray absorption spectroscopy and photoelectron spectroscopy has been applied.

NEXAFS spectra of all samples were recorded at the $\text{Cu L}_{2,3}$ absorption edges at the Russian-German beamline at the BESSY II (Berlin, Germany).

The comparison of the $\text{Cu L}_{2,3}$ NEXAFS spectra of samples obtained by different temperature treatment with the reference compounds and principal component analysis of spectra has shown that: 1. samples synthesised at temperature of about 150°C show structural disorder that gives difficulties in the interpretations; 2. samples synthesised at temperature between 300 and 500°C show the presence of compounds of copper corresponding to CuO phase that is in agreement with the results of XPS; 3. samples synthesised at temperature of about 700°C have a signatures of two phases formation: CuO and a metal copper.

5P140

Electronic structure of CdO studied by soft X-ray spectroscopyIN Demchenko,^{1,2,3} JD Denlinger,² M Chernyshova,⁴ KM Yu,² D Speaks,^{2,5} P Olalde-Velasco,⁶ WC Stolte,^{1,2} O Hemmers,⁷ W Walukiewicz,² A Derkachova,³ K Lawniczak-Jablonska³¹Department of Chemistry, UNLV, Las Vegas, NV, United States; ²ALS, LBNL, Berkeley, CA, United States; ³Institute of Physics PAS, Warsaw, Poland; ⁴Institute of Plasma Physics and Laser Microfusion, Warsaw, Poland; ⁵Department of Materials Science and Engineering, UC, Berkeley, CA, United States; ⁶Instituto de Ciencias Nucleares, UNAM, Distrito Federal, Mexico; ⁷Harry Reid Center for Environmental Studies, UNLV, Las Vegas, NV, United States

We present X-ray absorption spectroscopy (XAS) and resonance inelastic X-ray scattering (RIXS) measurements on CdO, in which we address controversial fundamental issues such as the band gap values for CdO. *Ab initio* theoretical calculations were performed and compared to the experimental results, using the FEFF code. The calculated PDOS semi-quantitatively describes all of the features corresponding to occupied and unoccupied states of the investigated films. Overlapping of the XAS spectrum with RIXS makes it possible to estimate both the direct ~2.4 eV and the indirect ~0.9 eV band gap values. The obtained results are consistent with the theoretical/experimental ones presented in the literature and our own optical absorption results.

5P141

Full multiple scattering analyses of XANES and X-ray emission studies of AgCl near the Cl K-edgeWC Stolte,^{1,2} IN Demchenko,^{1,2,3} O Hemmers⁴¹Department of Chemistry, UNLV, Las Vegas, NV, United States; ²ALS, LBNL, Berkeley, CA, United States; ³Institute of Physics PAS, Warsaw, Poland; ⁴Harry Reid Center for Environmental Studies, UNLV, Las Vegas, NV, United States

A detailed interpretation of X-ray absorption near edge structure at the K-edge of chlorine in AgCl within the *ab initio* RSM formalism (FEFF8 code), with many-body effects incorporated in terms of final-state potentials and complex energy-dependent self-energy, will be shown. Based on real space MS theory we were able to interpret the experimental spectra in terms of local geometrical and electronic structures. In order to probe the bulk-sensitive occupied valence band electronic structure, near-threshold excitation the chlorine-K emission spectra were recorded for AgCl. Calculated PDOS semi-quantitatively describes all features corresponding to occupied and unoccupied states of the investigated sample.

5P142

Prebiotic photocatalytic reactivity of formamide in presence of TiO₂R Saladino,² JR Brucato,¹ A Fort,² A De Sio,³ E Pace,³ L Gambicorti,⁴ L Tozzetti,³ A Grilli,⁵ A Raco⁵¹INAF - Osservatorio Astrofisico di Arcetri, Firenze, Italy; ²Università della Tuscia, Viterbo, Italy; ³Dip. Fisica e Astronomia, Università di Firenze, Firenze, Italy; ⁴CNR-INO, Firenze, Italy; ⁵INFN, Lab. Nazionali di Frascati, Roma, Italy

Laboratory experiments show that different chemical-physical mechanisms are responsible for the richness of molecules observed in space. Surface catalysis at low temperature by dust is necessary to justify the presence of, e.g., H₂, H₂O or CO₂, as demonstrated experimentally. However, to describe the presence of more complex molecules or radicals and even organic refractory material, irradiation processes due to ions and UV photons are required. Syntheses of organic molecules, occurring in space, were performed in laboratory following different strategies. Prebiotic reactions were studied by simulating the environments found on the early Earth and in space. Formamide is confirmed to be a promising route to understand the first chemical steps that brought simple C-bearing molecules towards largely complex mixtures of bio-macro-molecules. A large suite of pyrimidines (including cytosine and uracil) and purines were synthesized at 160°C using formamide in presence of cosmic-dust analogue silicates. In this work the reactivity of the formamide in presence of titanium dioxide is studied. TiO₂ is an important photo-catalytic material, thus we have developed an experimental protocol to investigate the role of UV radiation on bio-molecules formation. We irradiated with UV light at the SOURCE beamline at the DAΦNE-L laboratory (INFN), mixtures of formamide with two mineral forms of titanium dioxide: anatase and rutile. Results on photo-chemical synthesis will be presented and compared with those on thermal synthesis of biomolecules.

5P143

Soft X-ray absorption studies of Prussian blue analogues as electrode materials for Li-ion battery

D Asakura,¹ M Okubo,¹ T Kudo,¹ HS Zhou,¹ I Honma,² JL Chen,³ JH Guo,³ FMF de Groot⁴

¹Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan; ²Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Miyagi, Japan; ³Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, United States; ⁴Department of Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan, Utrecht, Netherlands

Prussian blue analogues (PBAs) are promising candidates for electrode materials of Li-ion battery [1] because of the porous coordinating and rich physical properties [2]. However, the electronic structure change of PBA frameworks have never been investigated during the Li-ion insertion/extraction. It is highly important to element-selectively investigate the electronic structure. We have studied the electronic structure of $\text{Li}_x\text{K}_{0.14}\text{Mn}_{1.4}\text{Fe}(\text{CN})_6 \cdot 6\text{H}_2\text{O}$ PBAs ($0 \leq x \leq 0.9$) by means of soft X-ray absorption spectroscopy (XAS). The Mn $L_{2,3}$ -edge XAS showed the multiplet structure of Mn^{2+} ($3d^5$) high-spin state regardless of the Li concentrations. The Mn atoms are not redox-active. On the other hand, considering the Fe $L_{2,3}$ -edge XAS of related cyanides [3], the multiplet structure for the Fe $L_{2,3}$ -edge XAS of the present PBAs should gradually change from Fe^{3+} ($3d^5$) low-spin to Fe^{2+} ($3d^6$) low-spin states in going from the Li-ion extracted to inserted states. The Fe $3d_{t_{2g}}$ down-spin state is the frontier orbital and the Fe atoms are redox-active in this material.

[1] M. Okubo *et al.*, submitted.

[2] S. Ohkoshi *et al.*, *Coord. Chem. Rev.* **249**, 1830 (2005).

[3] R. K. Hocking *et al.*, *J. Am. Chem. Soc.* **128**, 10442 (2006).

5P144

Speciation of arsenic in the thermally-stabilized photoelectronic industrial sludge

CY Liao,¹ HP Wang,^{1,2} YL Wei³

¹Department of Environmental Engineering, National Cheng Kung University, Tainan, Taiwan; ²Sustainable Environment Research Center, National Cheng Kung University, Tainan, Taiwan; ³Department of Environmental Science and Engineering, Tunghai University, Taichung, Taiwan

Arsenic containing photoelectronic sludges collected from the southern Science Park of Taiwan were thermally stabilized at the temperature range of 973-1373 K. To better understand the effectiveness of the thermal stabilization process, speciation of arsenics in the stabilized sludges has been studied by X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS). The least-squares fitted XANES spectra indicate that As_2O_5 and $\text{As}(\text{V})_{\text{ads}}$ are the main arsenic species in the sludges. The $\text{As}(\text{V})_{\text{ads}}$ species are not perturbed during the thermal stabilization at 973-1373 K. By EXAFS, the coordination numbers and bond distances of the first As-O shell are 5.9-6.8 and 1.68-1.69 Å, respectively. Notably, formation of crystalline whitlockite ($\text{Ca}_3(\text{PO}_4)_2$) is observed, which may account for the reduction of the leachable arsenics in sludges.

5P145

Fate of chromium in the ash and sludge wastes plasma melting process

YJ Tuan,^{1,2} HP Wang,^{1,2} JE Chang,^{1,2} CC Chao,² CY Liao¹

¹Department of Environmental Engineering, Cheng Kung University, Tainan, Taiwan; ²Sustainable Environment Research Center, Cheng Kung University, Tainan, Taiwan

Leachable chromium from the laboratory waste incineration ashes and wastewater sludges was found excess the limit of the Taiwan EPA toxic characteristic leaching procedure (TCLP) concentration (5 mg/L). By X-ray absorption (near edge structure (XANES) and extended X-ray adsorption fine structure (EXAFS)) spectroscopy, it is found that the main chromium species in the fly ashes and dried sludge are $\text{Cr}(\text{NO}_3)_3$ and $\text{Cr}(\text{OH})_3$. At the temperatures of 1673-1773 K, under the reducing environment, the ash, sludge, and waste glass (for a better vitrification) (1:1:2) are thermally stabilized in the plasma melting chamber. To track fate of chromium, four representative slags sampled from the melting chamber at the temperature zones between 1073 and 1773 K have also been studied by XRD, XANES, and EXAFS. At the 1773 K zone, low-oxidation state chromium [Cr(0) (8%) and Cr(II) (13%)] is found in the slag. Near the bottom of the chamber at 1073 K, Cr(0) may be oxidized to form Cr(III). Note that in the slag, chromium is encapsulated in the SiO_2 matrix, which also causes a reduction of the leachable concentration of chromium from the slag by at least 90%. The Cr-O-Si species with bond distances of 2.00 [Cr-O], 2.74 [Cr-O-Cr] and 3.12 Å [Cr-O-Si] are also observed by EXAFS.

5P146

Chemical substitution effect on the electronic structure of CoSi studied by X-ray absorption spectroscopy

CC Hsu,¹ CL Dong,¹ JL Chen,² YS Liu,² CL Chang,² YK Kuo,³ CS Lue⁴¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Department of Physics, Tamkang University, Tamsui, Taiwan; ³Department of Physics, National Dong Hwa University, Hualien, Taiwan; ⁴Department of Physics, National Cheng Kung University, Tainan, Taiwan

We report the effects of Al and Ge partial substitution for Si on the electronic structure of thermoelectric materials in the binary compound cobalt monosilicides, $\text{CoSi}_{1-x}\text{Al}_x$ ($0 \leq x \leq 0.12$) and $\text{CoSi}_{1-x}\text{Ge}_x$ ($0 \leq x \leq 0.15$). The correlations between electronic structure and the thermoelectric properties were investigated by means of X-ray absorption near edge structure (XANES) spectroscopy. As partially substituting Al onto Si sites in CoSi, the hole was gradually carried into the system. It was found for $x \leq 0.05$, the hole was not carried into the Co 3d states. However, the hole was carried into the Co 3d states upon further Al substitution for $x \geq 0.05$. This leads to the sign of Seebeck coefficient changes from negative to positive. In the system with different Ge substitution, the charge transfer between Co 3d and Ge 4p were observed and affect the density of states at Fermi level, which makes change of Seebeck coefficients (S). The Co K-edge of XANES shows that increased Al and Ge concentration do not affect the absorption intensity. It is also observed that the valence of Co remains unchanged with the doping. The improvement of the thermoelectric properties were interpreted on the basis of the variation of electronic structure induced by the chemical substitution.

5P147

Electronic structure change of Prussian blue analogue $\text{K}_2\text{Mn}[\text{Mn}(\text{CN})_6]$ during electrochemical K-ion extraction

D Asakura,¹ M Okubo,¹ T Kudo,¹ HS Zhou,¹ JL Chen,² JH Guo²¹Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan; ²Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, United States

Prussian blue analogue (PBA) $\text{K}_2\text{Mn}^{\text{II}}[\text{Mn}^{\text{II}}(\text{CN})_6]$ with the Mn-CN-Mn frameworks [1] is a possible candidate for electrode materials of Li-ion batteries. The $[\text{Mn}(\text{CN})_6]^{4-}$ defects in $\text{K}_2\text{Mn}[\text{Mn}(\text{CN})_6]$ are very few, which is advantageous to achieve a high charge/discharge capacity. Furthermore, if all the K-ions could be electrochemically extracted, both of the Mn sites would be redox-active and the electronic structure must change drastically. In that sense, we have been focusing K-ion extraction from $\text{K}_2\text{Mn}[\text{Mn}(\text{CN})_6]$ in this study. The synthesis of $\text{K}_2\text{Mn}^{\text{II}}[\text{Mn}^{\text{II}}(\text{CN})_6]$ was carried out according to the procedure in Ref. [1]. The CHN elemental analyses revealed that the hydrogen content was less than 0.3 wt%. Thus, the amount of zeolitic water in $\text{K}_2\text{Mn}[\text{Mn}(\text{CN})_6]$ was very few, and the $[\text{Mn}(\text{CN})_6]^{4-}$ defects were suppressed completely, which well agrees with the previous report. The electrochemical K-ion extraction carried out under a galvanostatic condition (constant current of 30 mA/g) showed two K-ion extraction voltages [3.1 and 3.6 V vs. Li/Li⁺], which clearly suggests the oxidation reaction of the Mn(II)-ions with two coordination environments [2]. Furthermore, the K-ions were almost extracted from the host. In this study, we will present the Mn 3d electronic structure change during the K-ion extraction reaction probed by electron spectroscopy. The soft X-ray absorption at the Mn $L_{2,3}$ -edge and X-ray photoemission results during the K-ion extraction will be discussed. [1] J.-H. Her et al., *Inorg. Chem.* **49**, 1524 (2010). [2] D. Asakura et al., in preparation.

5P148

The F 1s NEXAFS spectrum of polytetrafluoroethylene

E Kobayashi,¹ K Okudaira,² T Okajima¹¹Kyushu Synchrotron Light Research Center, Tosu, Japan; ²Graduate School of Science and Technology, Chiba University, Chiba, Japan

We have measured near-edge X-ray absorption fine structure (NEXAFS) spectra of polytetrafluoroethylene (PTFE) sheets and PTFE/Cu thin films using the total fluorescence yield and the total electron yield, and calculated the NEXAFS spectra of PTFE using density functional theory (DFT). The NEXAFS spectrum of the PTFE sheets is different to that of the PTFE/Cu thin films. This result is discussed in terms of the electronic and structural properties of PTFE.

5P150

XAS study of Cr transformation in incinerator fly ashes after firing process

YL Wei,¹ HC Wang,¹ CC Hsu,¹ YS Peng,¹ HP Wang²¹Department of Environmental Science and Engineering, Tunghai University, Taichung City, Taiwan; ²Department of Environmental Engineering, Cheng-Kung University, Tainan City, Taiwan

Heating Cr-containing fly ashes to lower temperatures leads to a less chemical reduction of Cr(VI) that is 1000 times more toxic than Cr(III). Most sorbed Cr(VI) was effectively reduced to Cr(III) in fly ashes after heating to 1100 °C whereat the sample was held for 2 hours, as revealed by the almost disappeared preedge peaks at 5991-5996 eV of Cr K-edge XANES spectra. Water soluble, toxic CaCrO_4 was formed due to the chemical reaction between Cr(VI) and calcium oxide component of fly ash when the Cr-containing fly ashes were heated to 100 and 500 °C, based on the XANES comparison between samples and references. SEM morphologies show the occurrence of ash sintering and/or melting at 900 °C and 1100 °C, thereby enhancing the chemical reaction between chromium compounds and fly ash components due to an improved fluidity and mixing.

5P152

XAS study on the removal of CMP nanoparticles with copper ionsYL Wei,¹ KW Chen,¹ CC Hsu,¹ YS Peng,¹ HP Wang²¹Department of Environmental Science and Engineering, Tunghai University, Taichung City, Taiwan; ²Department of Environmental Engineering, Cheng-Kung University, Tainan City, Taiwan

An attempt was made to reduce the turbidity caused by nanoparticles in the wastewater collected from a high-tech plant by way of adding proper amount of Cu-containing wastewater sampled from a semiconductor manufacturing company. Because of the electrostatic attraction principle to agglomerate the SiO₂ nanoparticles, the turbidity of CMP wastewater reduces from about 60 to 0.60 NTU. After the agglomeration of nanoparticles with added copper ions, conventional wastewater treatment techniques can be used to remove the agglomerates. XAS was used to investigate the species change of the added copper ions in the SiO₂ nanoparticles aggregates. The XANES results show that copper ions were chemically reduced after the agglomeration.

5P153

Electronic properties of singlet dioxygen as a ligandD Covelli,¹ P Kennepohl¹¹Department of Chemistry, The University of British Columbia, Vancouver, BC, Canada

In collaboration with the Crudden group at Queens University, our group has recently characterized several Rh(I)-O₂ complexes using X-ray Absorption Spectroscopy (XAS). These complexes appear to have dioxygen bound to the metal centre without concomitant oxidation of the Rhodium.¹ The complexes were found to exhibit a new bonding motif which was best described by Rh{¹O₂} adducts.¹ The Whittlesey group at the University of Bath, has recently synthesized a ruthenium dioxygen species which contains an unusually short O-O bond distance, similar to the rhodium complexes.² Therefore, we have been studying a set of ruthenium compounds synthesized in the Whittlesey group using both Ru K and Ru L_{2,3} edge XAS to investigate the bonding of the O₂ to the ruthenium centres. Semi-quantitative spectroscopy demonstrating the differences between the single and triplet species will be discussed and correlated with expected reactivity of the various compounds.

[1] J.M. Praetorius, D.P. Allen, R.Wang, J.Webb, F.Grein, P.Kennepohl, and C.M. Crudden, *J.Am.Chem.Soc.*, **2008**, 130[12] 3724-3725

[2] L. Jonas L. Hällner, E. Mas-Marzá, A. Moreno, J.P. Lowe, S.A. Macgregor, M.F. Mahon, P.S. Pregosin, and M.K. Whittlesey; *J.Am.Chem.Soc.*, **2009**, 131[28] 9618-9619

5P156

XAFS analysis of Zn_{1-x}Mn_xO nanopowders: effects of concentration and processing temperature on secondary phase formation and magnetismMW Murphy,¹ L Bovo,² MJ Ward,¹ L Liu,¹ L Armelao,² TK Sham¹¹Department of Chemistry, University of Western Ontario, London, ON, Canada; ²Department of Chemistry, University of Padova, Padua, Italy

Much of the recent effort toward ferromagnetic (FM) semiconductor devices has been focused on the synthesis and characterization of transition metal (TM) doped III-V and II-VI materials, with prominent interest in Zn_{1-x}Mn_xO due to a proposed Curie temperature above room temperature. However, much controversy surrounds these systems as researchers report conflicting observation of both room temperature FM and anti-FM or paramagnetism in Zn_{1-x}Mn_xO. Additionally, it is still unclear whether the FM is intrinsic (carrier-induced) or due to Mn-related secondary phases. Therefore, it is of great importance to find the relationship between the local environment of the Mn and the magnetic properties of the system. X-ray absorption fine-structure (XAFS), X-ray excited optical luminescence (XEOL), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and magnetic susceptibility measurements have been used to characterize a series of Mn doped ZnO nanopowders grown by sol-gel methods with varying Mn concentration and processing temperature. We show that the Mn L_{3,2}-edge and O K-edge are more effective than the Mn K-edge at determining secondary phase formation, which is more prevalent at higher Mn concentrations and processing temperatures. Additionally, the photoluminescence emissions are strongly quenched with increased Mn concentration. Correlations are also made between the composition and observed magnetic properties.

5P157

XAFS analysis of Zn_{1-x}Cu_xO nanopowders: effects of concentration and processing temperature on secondary phase formationMW Murphy,¹ L Bovo,² L Armelao,² TK Sham¹¹Department of Chemistry, University of Western Ontario, London, ON, Canada; ²Department of Chemistry, University of Padova, Padua, Italy

Copper based catalysts are used in a wide variety of industry processes. Cu doped ZnO is a promising candidate for steam reforming of methanol which has the potential for large scale production of H₂ for fuel cells. For catalytic applications the location, phase and oxidation state of the copper in the ZnO is of great interest. X-ray absorption fine-structure (XAFS) were carried out at the Cu K-edge and L_{3,2}-edge, O K-edge and Zn L_{3,2}-edge on a series of copper doped ZnO nanoparticles prepared by sol-gel methods at a variety copper concentrations and processing temperatures. The results indicate that at low processing temperature the system is a mixture of CuO and ZnO. However, there is an increased ratio of CuO:ZnO in the bulk than at the surface. At a processing temperature of 800°C the copper is begins to incorporate into the ZnO and occupies a Zn vacancy (Cu_{Zn}) resulting in a Zn_{1-x}Cu_xO wurtzite phase alloy.

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Local structure of photoexcited metal complexes refined by quantitative XANES analysis

G Smolentsev,¹ J Lockard,² L Chen,² S Canton,³ V Sundstrom¹

¹Department of chemical physics, Lund University, Lund, Sweden; ²Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, United States; ³MAX+lab, Lund University, Lund, Sweden

Knowledge of the local structure of metal complexes in the photoexcited state is important to understand and visualize the mechanisms of photochemical reactions and subsequently to improve materials for dye sensitized solar cells and photocatalysts for hydrogen production. Pump-and-probe X-ray absorption spectroscopy also known as X-ray transient absorption allows to measure spectra with time-resolution around 100ps. We have developed the approach to quantitatively analyze these spectra and to extract structural information [1]. This approach is based on the fitting of the difference between spectra of complex in the photoexcited and ground state and combines multidimensional interpolation of spectra as a function of structural parameters, muffin-tin full multiple scattering or non-muffin-tin finite difference method calculations of XANES spectra. Application of the technique to Cu diimine, Pt-Pt pyrazolate bridged and bimetallic Ru-Co complexes are presented. Its advances, possibilities and limitations are discussed.

[1] Smolentsev et al *J. Phys. Chem. A* (2008) 112, 5363

5P159

X-ray absorption study of silicon carbide thin film deposited by pulsed laser deposition

G Monaco,^{1,5} M Suman,¹ D Garoli,^{2,3,4} M Pelizzo,^{1,5} P Nicolosi^{1,5}

¹Laboratorio LUXOR, CNR-IFN, Padova, Italy; ²Physical Department "G. Galilei", University of Padova, Padova, Italy; ³LANN Laboratory for Nanofabrication of Nanodevices, Padova, Italy; ⁴CNR-ICIS, Padova, Italy; ⁵Department of Information Engineering, University of Padova, Padova, Italy

Silicon Carbide (SiC) is an important material for several application ranging from electronics to Extreme UltraViolet (EUV) space optics. Crystalline cubic SiC (3C-SiC) has a low band gap (2.36 eV) and it a promising material to be used in high frequency and high energetic electronic devices. We have deposited by means of Pulsed Laser Deposition (PLD) different SiC films on Sapphire and on Silicon substrates both at mild (650°C) and a room temperature. The resulted films have different structures such as: oriented polycrystalline, polycrystalline and amorphous which have been studied by means of X-ray absorption spectroscopy (XAS) near the Si L_{2,3} edge and the C K edge and by the analysis of the valence band. The "non-standard" samples obtained by PLD have shown spectra which are different among the grown films, some of them showing typical 3C-SiC absorption structure, but also the presence of some Si-Si and graphitic bonds.

5P160

Extended X-ray absorption fine structure calculations for copper using the finite difference method

JD Bourke,¹ CT Chantler¹

¹School of Physics, University of Melbourne, Parkville, Victoria, Australia

X-ray Absorption Fine Structure (XAFS) is calculated for copper using the cluster based Finite Difference Method for Near-Edge Structure (FDMNES). This approach is conventionally used to produce high accuracy XAFS theory in the near edge region [1, 2], however we demonstrate that it can be readily extended to encompass an energy range of more than 1.5keV from the K absorption edge. Such calculations require extensions to FDMNES to account for thermal effects, in addition to broadening effects due to inelastic processes [3]. Extended calculations beyond the range of XAFS also require consideration of technical constraints such as cluster sizes and densities. We find that with our approach, we are able to produce accurate theory ranging from the absorption edge, to the smooth atom-like region at high energies, with a single consistent model that is free from any fitting parameters.

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[3] J. D. Bourke, C. T. Chantler, and C. Witte, *Phys. Lett. A* **360**, 702 (2006)

5P161

Novel measurement of low energy electron inelastic mean free paths in copperJD Bourke,¹ CT Chantler¹¹School of Physics, university of Melbourne, Parkville, Victoria, Australia

We present a new approach for determining the Inelastic Mean Free Path (IMFP) of electrons in various materials, using analysis of X-ray Absorption Fine Structure (XAFS) measurements. Our procedure involves the fitting of theoretical XAFS spectra produced using the finite difference method to high accuracy XAFS measurements obtained with the X-ray extended range technique [1, 2]. We apply our technique to copper and find that we can distinguish between different IMFP calculations at low energies. Since our approach is particularly suited to the low energy regime (below 100eV) [3], this gives it a distinct advantage over other measurements and calculations, which typically possess high uncertainties or require severe approximations at these energies.

[1] J. L. Glover, C. T. Chantler, Z. Barnea, N. Rae, C. Q. Tran, D. C. Creagh, D. Paterson, and B. B. Dhal, *Phys. Rev. A* **78**, 052902 (2008)

[2] C. T. Chantler, C. Q. Tran, Z. Barnea, D. Paterson, D. Cookson, and D. X. Balaic, *Phys. Rev. A* **64**, 062506 (2001)

[3] J. D. Bourke, C. T. Chantler, and C. Witte, *Phys. Lett. A* **360**, 702 (2006)

[4] J. D. Bourke, C. T. Chantler, PRL submission in review

5P162

Ab initio study of core-level X-ray photoemission spectra from transition metal compoundsM Takahashi¹¹Gunma University, Kiryu, Gunma, Japan

We have developed a method of the ab-initio calculation for the core-level X-ray photoemission spectroscopy (XPS). The theory used by Feldkamp and Davis[1] is combined with an ab-initio band structure calculation. We carry out the band structure calculation within the local density approximation to obtain the one-electron states and their wavefunctions in the ground state. Next, we consider a system of supercells containing one core-hole per cell to simulate the photo-excited state. The core hole is introduced by removing an electron from the core state. In this system, we carry out the band structure calculation to obtain the one-electron states and their wavefunctions. The state self-consistently obtained in this system can be considered as the fully screened state. Finally, we calculate the XPS spectra by evaluating the overlaps between the photo-excited states and the ground states. In this method, the effect of core-hole potential and also that of electron-electron interaction are taken into account in the one-electron states within LDA. We apply the procedure to the analysis of the core-level XPS in transition metals and their metallic compounds. We obtain the spin-resolved 3s core-level XPS spectra in good agreement with experiments for iron, nickel, and cobalt[2]. The spectral shape are quite different for different spin channels. We discuss the screening behaviors with relating to the electronic structure in the ground state and explain the behaviors of the 2p and 3s XPS spectra in the transition metals and their metallic compounds in terms of the difference in the one-electron states screening the core-hole potential.

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[2] M.Takahashi and J.Igarashi, PRB81, 035118 (2010).

5P163

The local atomic and electronic structure of Ti-bearing geological materials of spinel group: XANES studyI Rodina,¹ A Kravtsova,¹ A Soldatov,¹ A Berry,² G Smolentsev¹¹Southern Federal University, Rostov-on-Don, Russian Federation; ²Imperial College London, London, Great Britain

The local atomic structure of Ti-bearing geological materials of spinel group was studied. The X-ray absorption spectrum near Ti- K edge in Ti-bearing spinel was recorded at the Photon Factory, KEK (Japan). The theoretical simulating of the spinel XANES spectra was made for two models: 1) $\text{Ni}_{2.62}\text{Ti}_{0.69}\text{O}_4$; 2) $\text{Ni}_{2.42}\text{Ti}_{0.74}\text{Si}_{0.05}\text{O}_4$ (silicon atoms occupy the titanium atoms site) [1]. The theoretical XANES analysis makes it possible to determine the most suitable model of the local structure around Ti atoms. The theoretical calculations of XANES spectra were performed on the basis of the finite difference method. All calculations used the real Hedin- Lundqvist exchange potential. The electronic structure of spinel was investigated by analyzing the distribution of the partial densities of electron states

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5P164

Correlation of spectral features in the O K edge and $L_{2,3}$ spectra of amorphous SiO_2 based on the application of the charge transfer multiplet (CTM) formalism

G Lucovsky,¹ L Miotti,¹ K Paz Bastos¹¹Physics, NC State Univ, Raleigh, NC, United States

In SiO_2 4-fold coordinated Si bonded to 2-fold coordinated O in a bent 3-atom group has 3d t_{2g} symmetries [1], constraining dihedral bond angles bringing O-atoms [2]. Analysis of O K edge spectra identify conduction band states with 3s symmetries at the band edge, and stronger 3d states at higher energy. Their relative energies are the same as band edge states in transmission and reflectivity studies [3]. This similarity derives from O 1s core hole localization, and coherent processes whereby core states are filled by electrons from valence band O 2p s-bonding, p-bonding, or p-non-bonding states. There is also a one-to-one correspondence between Si 3s and Si 3d features in O K edge and Si $L_{2,3}$ spectra. Studies of $L_{2,3}$ transitions by electron energy loss spectroscopy (EELS) do not detect Si 3s features in the 100 to 104 eV regime; however, EELS studies of the O K edge displayed lower energy features, but their symmetries were not specified. Analysis of O K and $L_{2,3}$ spectra are based on the CTM formalism. The ground state is $\text{Si}2p^63d^0\bar{\underline{L}} + \text{Si}2p^63s^0\bar{\underline{L}}$, where $\bar{\underline{L}}$ indicates a coherent process in which Si 2p core level holes are neutralized by electrons from the three O 2p states noted above. Ground states have ¹A symmetries [4]. Excited states are $\text{Si}2p^53d^1\bar{\underline{L}} + \text{Si}2p^53s^1\bar{\underline{L}}$ with ¹F and ¹P symmetries, respectively. Degeneracies are lifted by different J values associated with the orbital angular momentum. Defect state pre-edge spectra are assigned to an O-atom vacancy represented by a high spin Si d^2 state employing Tanabe-Sugano energy level diagrams.

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5P165

Sum rules for local fields in dielectric response in solids

EL Shirley¹¹Optical Technology Division, NIST, Gaithersburg, MD, United States

Understanding the response of atoms, molecules and solids to disturbances, including their polarizability and absorption properties in the deep ultraviolet, requires characterization of their frequency-dependent dielectric response. The f-sum rule, Kramers-Kronig relations and completeness relations all provide constraints on various frequency or energy moments of the dielectric response of a system, in terms of how the electronic charge density is affected in the vicinity of a local potential disturbance. In this work, I shall show how the variations in density within a bulk system, such as between low densities in interstitial regions and high densities in bonds between atoms, affects the dielectric response on the 0.1 nm length scale. In this regard, I show that the effects of density variations is captured reasonably well by sum rules that permit one to determine many aspects of dielectric response through knowledge of only ground state properties of one's system, the charge density in particular. The frequency-dependent dielectric response can therefore be easily modeled in a fashion that is readily exploited in calculations of electron state lifetime widths, so that the widths of electron states probed by photoemission and/or near-edge spectroscopies are reasonably well reproduced. This will be demonstrated in a range of semiconductors and insulators, whereas the concepts presented here should apply equally well to liquids and amorphous solids.

5P166

Next generation instrumentation for ambient pressure PES and HAXPES

M Lundwall¹¹VG Scienta AB, Uppsala, Sweden

We report on the recent development of instrumentation for ambient pressure PES and HAXPES. The ambient pressure PES set-up is a versatile instrument for high throughput measurements which is based on a Scienta R4000 with the addition of a HiPP pre-lens for high pressure measurements. This allows both traditional XPS and UPS as well as spectromicroscopy with better than 15 micron resolution, and even ± 13 degree wide angle ARPES in ambient pressure conditions. For high transmission and HAXPES experiments we show recent results from a newly developed extreme wide angle lens spectrometer showing a parallel angular resolved range of 60 degrees. Besides increasing the throughput compared to standard analyzers the extreme wide angle lens also increases the available angular resolved range to the full HAXPES kinetic energy region.

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The cylindrical sector analyzer: HAXPES Instrumentation up to 15 keVM Merkel,¹ M Escher,¹ N Weber¹¹FOCUS GmbH, Huenstetten, Germany

HAXPES gains momentum as a new nanoanalytical method more and more. The availability of a growing number of suitable high energy synchrotron beam lines is demanding strongly for dedicated instrumentations. The FOCUS HV-CSA fulfills the requirements imposed by the XRD and HAXPES techniques at the same time. This analyzer of the cylindrical sector type is a very compact and highly efficient approach for this kind of electron spectroscopy. It is capable to handle routinely kinetic energies up to 15 keV and down to a few eV with the same analyzer setup and power supply. Because of its compact design it is very suitable to be integrated e.g. into existing or planned X-ray diffraction setups. This combination of the widely used diffraction method for structural analysis and/or the X-ray absorption spectroscopy with high energy photoelectron spectroscopy for chemical analysis is a very promising approach for material research at a number of synchrotron beam lines. It opens up new possibilities in terms of non destructive but bulk sensitive material research. We will describe the development and use of a new 2D event counting detector for parallel data acquisition also. By means of this new detector the measurement speed is increased to overcome the restrictions imposed by the low photo ionization cross sections at high kinetic energies. Using the whole dispersion plane of the analyzer it opens up more flexibility for the optimization of energy resolution and transmission at the same time. Typical results demonstrating the recent performance of the whole setup are shown.

5P168

Polarization-dependent hard X-ray photoemission spectroscopy: probing orbital contributions of conduction electrons in solidsA Sekiyama,^{1,2} J Yamaguchi,¹ A Higashiya,^{2,3} M Obara,¹ H Sugiyama,¹ MY Kimura,¹ S Suga,^{1,2} S Imada,⁴ IA Nekrasov,⁵ M Yabashi,^{2,6} K Tamasaku,² T Ishikawa²

¹Division of Materials Physics, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka, Japan; ²Spring-8/RIKEN, Sayo, Hyogo, Japan; ³Industrial Technology Center of Wakayama Prefecture, Wakayama, Japan; ⁴Department of Physical Sciences, Ritsumeikan University, Kusatsu, Shiga, Japan; ⁵Institute of Electrophysics, Russian Academy of Sciences-Ural Division, Ekaterinburg, Russian Federation; ⁶Spring-8/JASRI, Sayo, Hyogo, Japan

We have newly developed a method to study linear polarization-dependent hard X-ray ($h\nu \sim 8$ keV) photoemission, by which the orbital contributions in the valence band in solids can be probed due to the strong orbital dependence of photoelectron angular distribution. We have applied this technique to polycrystalline gold and silver in the same column in the periodic table with nominally filled d orbitals [1]. Rather contrary to common expectation, it is found that the 5d orbital electrons contribute prominently to the conduction electrons in gold, while the conduction electrons in silver are to some extent free-electron-like with negligible 4d contribution, which would be related to the well-known fact that gold is more stable than silver in air. From comparison between the experimental and computational data, we conclude that the 4d electron correlation effects are essential for the conduction electron character in silver.

[1] A. Sekiyama et al., New J. Phys. in press (2010).

5P169

The high resolution online grating spectrometer at FLASHG Brenner,¹ S Kapitzki,¹ M Kuhlmann,² E Plönjes,¹ K Tiedtke¹¹DESY, Hamburg, Germany; ²Cells-Alba, Barcelona, Spain

An new online high resolution grating spectrometer has been set up at the Free Electron Laser FLASH at DESY in Hamburg and is currently under commissioning. This new photon diagnostic device allows to parasitically measure the spectral distribution of the laser pulses on a shot to shot basis and therefore giving additional spectral and temporal pulse information for user experiments and FEL operation. The spectrometer combines a mirror and two variable line spacing (VLS) gratings with blazed surface and is installed at the non-monochromized beamline branch at FLASH. In contrast to a standard grating the blaze angle is optimized for the zero order transferred to the experimental stations, leaving approximately 1 – 10 % intensity for recording the wavelength in the spectrometer. The detector, an intensified CCD camera imaging the dispersed beam on a Ce:YAG crystal, can follow the focal plane of the gratings covering a wavelength range from 6 – 60 nm. The resolving power of the spectrometer on the CCD is expected to range from 500 to 8000 depending on the FEL energy. First measurements concerning the optical performance of the mirror and the gratings as well as resolution tests of the VLS grating spectrometer will be presented and the results are compared with the design parameters.

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Development of a new high-yield and high-resolution spin- and angle-resolved photoelectron spectrometer

T Okuda,¹ K Miyamoto,¹ Y Takeichi,² K Kuroda,³ H Miyahara,³ A Kimura,³ A Kakizaki,² H Namatame,¹ M Taniguchi¹

¹Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Japan; ²Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan; ³School of Science, Hiroshima University, Higashi-Hiroshima, Japan

We have recently developed a new spin-polarized photoelectron spectrometer in which high efficient spin detector based on the spin dependent very low energy electron diffraction (VLEED) is combined with a high-resolution photoelectron analyzer [1]. Almost 100 times higher efficiency than conventional Mott type spin polarimeter and consequent high-energy and angular resolution in spin- and angle-resolved photoelectron spectroscopy (SARPES) have been achieved. Utilizing this high-yield spin detector, a new SARPES end-station is now under construction at the undulator beamline BL-9B in Hiroshima Synchrotron Radiation Center (HSRC). By the VLEED detector and a high-resolution ARPES spectrometer (R4000, SCIENTA) with 90° electron deflector, high-yield SARPES measurement with high energy- and angular-resolutions will be available. While at the beamline BL-19A in Photon Factory (PF), KEK, present high-resolution SARPES system will be upgraded to be able to perform a 3D spin analysis by applying two VLEED polarimeters. In the paper, performance of the new spin detector and the status of the new SARPES endstations will be presented. [1] T. Okuda, Y. Takeichi et al., Rev. Sci. Instrum. 79, 123117 (2008).

5P172

DEIMOS beam-line or soft X-ray dichroism at synchrotron SOLEIL

E Otero,¹ P Ohresser,¹ S Stanesco,¹ F Deschamps,¹ P Sainctavit,² F Scheurer,³ J P Kappler³

¹Synchrotron SOLEIL, Saint Aubin, France; ²IMPMC, CNRS, Université Pierre et Marie Curie, Paris, France; ³IPCMS, CNRS, Université Louis Pasteur, Strasbourg, France

DEIMOS (Dichroism Experimental Installation for Magneto-Optical Spectroscopy) is a new beam-line at the French synchrotron (SOLEIL) dedicated to the study of magnetic and electronic properties using polarized light. It is installed on the medium straight section I-07M of the SOLEIL storage ring. The X-ray source will be produced by 2 undulators allowing to cover the energy range from 350 to 2500 eV with variable polarization (rotatable linear or circular). The first undulator of the APPLE-II type will have a period of 52 mm, the second will be a hybrid undulator (permanent magnets and electromagnets) allowing a fast switching of the polarization. The two undulators will be used alternately according to the type of measurement requested. This beam-line is characterized by extreme sample environment, with very high magnetic fields (7T) and very large temperatures range (1.5K to 1000K). The scientific thematic thus accessible on DEIMOS will cover a broad panel from magnetic nanostructures, molecular magnets, spintronic to paleomagnetism. <http://www.synchrotron-soleil.fr/portal/page/portal/Recherche/LignesLumiere/DEIMOS>

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IR and X-ray simultaneous spectroscopy: a novel framework for time resolved simultaneous analysis of physical-chemical processes

A Marcelli,¹ W Xu,^{2,1} P Innocenzi,³ L Malfatti,³ D Hampai,¹ U Schade,⁴ Z Wu^{5,2}

¹INFN-Laboratori Nazionali di Frascati, Frascati (RM), Italy; ²Institute of High Energy Physics, Beijing, China; ³Laboratorio di Scienza dei Materiali e Nanotecnologie, Università di Sa, Alghero (SS), Italy; ⁴Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; ⁵NSRL, University of Science and Technology of China, Hefei, China

Synchrotron radiation facilities offer a great number of different opportunities to a wide and continuously increasing scientific community, delivering intense and brilliant photon beams with extremely high time and spatial resolution in a very broad spectrum from the far-IR up to the hard X-ray. Dozens of storage rings are now operational all around the world and in almost all facilities the state-of-the-art spectroscopic and scattering techniques are available. Many physico-chemical transitions, catalysis processes, metal-insulator transitions, etc. involving correlated changes of electronic and atomic structure can be investigated. However, the concurrent combination of an IR and X-ray simultaneous spectroscopic analysis may return unique information on different aspects of a process. Pioneering time resolved experiments combining X-ray and IR radiation were performed more than a decade ago (W. Bras, *et al.*, *Science* (1995) 267, 996). Nowadays the combination of experimental techniques is a clear trend (R.J. Davies *et al.*, *Macromolecules* (2006) 39, 4834 and M.A. Newton *et al.*, *Phys. Chem. Chem. Phys.* (2007) 9, 246) and although challenging, the strategy of a concurrent analysis is mandatory in frontier multi-disciplinary areas. Actually, new opportunities can be open such as the possibility to probe complex phenomena on a short time scale. The simultaneous combination of atomic or structural analysis with molecular analysis will offer immense rewards to materials science and will certainly improve the understanding of many fundamental processes. We present the design of a novel beamline combining both X-ray and IR SR beams and the expected performance for simultaneous spectroscopy on a third generation high brilliance SR source (A. Marcelli *et al.*, *Anal. Bioanal. and Chem.* (2010) in press)

5P174

Development of a blazed multilayer grating for the SXR rangeF Senf,¹ F Schaefers,¹ T Zeschke,¹ R Dietsch,² B Nelles³¹Helmholtz-Zentrum-Berlin (HZB-BESSY-II), Berlin, Germany; ²AXO Dresden GmbH, Heidenau, Germany; ³CARL ZEISS Optronics GmbH, Oberkochen, Germany

To cover the energy gap between the classical working ranges of gratings and crystals we developed and tested a high efficiency blazed grating with a multilayer coating for operation between 1 and 3 keV. Two stripes of the 610 l/mm grating have been deposited with Cr/C and Pd/B₂C multilayers, respectively, by magnetron sputtering and, for comparison, one stripe was coated with a conventional Au layer. No change of the surface topography, line density and blaze angle [1.37 degrees] due to the multilayer deposition was detected by AFM. The multilayer stack (40 bilayers) has been optimised for operation in 5th order. Theoretical studies using the BESSY-REFLEC program were done, which employs the software package DMLDBE /1/, which solves the Maxwell equations in differential form. The grating efficiency has been measured at KMC-1 and SXR optics beamlines using the BESSY reflectometer. The preliminary data show enhancement of higher orders, strongly dependent on energy, incidence angle and blaze angle. For comparison and to disentangle Bragg reflection and grating diffraction the reflectivity of two identical multilayer mirrors (witness samples) have also been determined.

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5P175

Liquid xenon scintillation detection with avalanche photodiodesA Ribeiro,¹ S Orrigo,¹ L Coelho,¹ L Fernandes,¹ E Aprile,² K Giboni,² J Lopes,^{1,3} J dos Santos¹¹Departamento de Física, Universidade de Coimbra, Coimbra, Portugal; ²Department of Physics, Columbia University, New York, NY, United States; ³Departamento de Física e Matematica, Instituto Superior de Engenharia de Coimbra, Coimbra, Portugal

Large area avalanche photodiodes (LAAPDs) have proven to be a good alternative to photomultiplier tubes (PMTs) in visible and VUV photon detection [1,2]. Within the context of the R&D for the XENON project [3] we are testing the operation of different types of LAAPDs in liquid xenon (LXe) for the detection of its 178 nm centered scintillation light. We have investigated the performance of 16 mm in diameter Advanced Photonix (API) and 10x10 mm² Hamamatsu LAAPDs immersed in LXe. Quantum efficiencies of 1.08 ± 0.05 and 0.80 ± 0.14 where measured for the API and Hamamatsu LAAPDs, respectively. Both LAAPDs can reach gains of several hundred, but gains of as low as a few tens may be sufficient to achieve good energy resolution. The overall performance of the LAAPDs in LXe scintillation detection will be presented.

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5P176

Towards diamond UV imaging photodetectorsA De Sio,¹ E Pace,¹ S Scuderi,² R Di Benedetto,² M Focardi¹¹Dip. di Fisica e Astronomia, Università di Firenze, Firenze, Italy; ²INAF – Osservatorio Astrofisico di Catania, Catania, Italy

The recent improvements achieved in the Homoepitaxial Chemical Vapour Deposition technique have led to the production of high quality detector-grade single-crystal diamonds. Diamond-based detectors have shown excellent performances in UV and X-ray detection, paving the way for applications of diamond technology to the fields of space astronomy and high-energy photon detection in harsh environments or against strong visible light emission. These applications are possible due to diamond's unique properties such as its chemical inertness and visible blindness, respectively. Actually, the development of linear array detectors represents the main issue for full exploitation of diamond detectors. Linear or bidimensional arrays are crucial for UV and VUV imaging applications. Problems related to pixel miniaturisation and signal read-out from many channels as well as off-chip electronic readout are the challenging steps making diamond technology ready for full exploitation in application such as synchrotron radiation, astronomy, photo-biology. This work will report on the development of imaging detectors made by our groups, starting from the material growth and characterisation, through the design, fabrication and packaging of pixel arrays, to their electro-optical characterisation in terms of UV sensitivity, uniformity of the response and to the development of an electronic circuit suitable to read-out very low photocurrent signals.

5P177

Development of angle-resolved time-of-flight electron-spectrometer using streak camera system

K Sato,¹ T Abukawa¹¹IMRAM, Tohoku University, Sendai, Japan

In recent years, a pulse nature of a synchrotron radiation has been utilized to investigate temporal phenomena of the matter. Time-resolved photoemission combined with pump laser system is one of the trends of the synchrotron facility. For the photoemission with a pulse probe light, a time-of-flight (TOF) detector is one of the choices among electron-spectrometers. For this purpose, we are developing a new TOF electron spectrometer using a streak camera system. The spectrometer consists of a one-dimensional entrance slits, focusing electron lens, sweep electrodes and a MCP screen. Utilizing an advantage of a time-resolution of the streak system (~ 10 ps), only 60mm drift length results an energy resolution of 1/1000 at the electron kinetic energy of 100eV. Thus, we can reduce the size of the TOF spectrometer by using the streak camera system in the present. Since the one-dimensional slits accept photoelectrons with angle of 30 degree, angular distributions of photoemission spectra can be displayed on the MCP screen. Details and the preliminary results will be presented.

5P178

New beamline proposal for complex nanosystems characterization at the Siberia-2 storage ring

VG Stankevich,¹ VG Nazin,¹ MB Tsetlin,¹ LL Lev,¹ AN Marchenkov,¹ AM Lebedev,¹ MN Mikheeva,¹ SN Ivanov,¹ YV Zubavichus¹¹Russian Research Center Kurchatov Institute, Moscow, Russian Federation

We report the design of a photo-electron spectroscopy station joined with a UHV modular nanotechnological complex «Nanofab-100» via a special sample-transmission system. The «Nanofab-100» presently consists of a robotic sample-handling chamber and an array of independent sample preparation and analysis modules. Operational modules include: plasma etching, laser ablation fitted with RHEED, focused ion beam milling and etching, focused ion beam implantation fitted with a scanning electron microscope and two multifunctional AFM modules. The new station's sample chamber will include a hemispherical analyser capable of doing angle-resolved measurements, whose energy resolution is better than 1 meV and angular resolution is better than 0.1 degrees. The synchrotron radiation is passed through a monochromator with the energy band between 25–1500 eV. Along with photoelectron spectra, absorption spectra will be measured as well. The sample chamber will also be equipped with a compact X-ray source and a monochromator. Samples in the chamber are positioned on a support, which is cooled by an autonomous refrigerator. A specially designed robotic load mechanism allows for a quick change of samples in the chamber. The proposed station is suitable for solving a wide range of problems in the area of surface physics and layered materials and structures, including epitaxial graphene and high-Tc superconductors.

5P179

Identification and treatment of an efficiency anomaly in a symmetrically ruled grating illuminated at normal incidence.

FE Vincent,¹ WM Harris,² LB Jaffel¹¹Institut d'Astrophysique de Paris, Paris, France; ²Department of Applied Science, UC Davis, Davis, CA, United States

The use of gratings for symmetric dispersion (symmetric blaze gratings) is an uncommon implementation but one that is employed in specialized astronomical instrumentation including dual order spectrograph and all-reflective spatial heterodyne spectrometers. These implementations require illumination at normal incidence, a configuration that is often not tested experimentally for commercial gratings where the desire for high efficiency in a single order is the primary goal. We report here experimental results of normal incidence dual-order efficiency testing of an Al-MgF₂ coated holographic grating with a square profile optimized to 121.6 nm. These tests revealed an anomaly that was sharply peaked at normal incidence and was not predicted by industry-standard theoretical models. The anomaly resulted in a 50% reduction in the efficiency into each of the ± 1 orders of the grating. Our mitigation strategy for this involved over-coating the grating using an optimized Al-MgF₂ mix developed by at the Goddard Space Flight Center for the UV gratings used in the Cosmic Origins Spectrograph. After re-coating the anomaly was eliminated, but at a cost of a reduction in the peak efficiency of the symmetric orders and an increase in grating specular (zero-order) reflection. We discuss the respective roles of the new coating characteristics and the effect of groove smoothing from repetitive overlays in the observed changes in the grating performance.

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Quantum Material Spectroscopy Center at the Canadian Light Source

S Gorovikov,¹ B Yates,¹ A Damascelli,^{2,3} H Davis,² R Reininger,⁴ K I Blomqvist,⁵ M Sigrist,¹ V Nagarkal,¹ S Chen,¹ E Hallin,¹ M de Jong¹

¹Canadian Light Source Inc., Saskatoon, SK, Canada; ²Departments of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada; ³AMPEL, University of British Columbia, Vancouver, BC, Canada; ⁴Scientific Answers and Solutions, Mount Sinai, NY, United States; ⁵Consultant, Sweden, Sweden

We report on the concept and design features of the Quantum Material Spectroscopy Center (QMSC), a state-of-the-art XUV and soft X-ray beamline facility currently under construction at the Canadian Light Source. The QMSC will operate within the photon energy from 15 to 1200 eV and is intended for spin- and angle-resolved photoemission spectroscopy (SARPES and ARPES). A distinctive feature of the QMSC is the combination of two independent end stations dedicated to SARPES and ARPES experiments with a unique source consisting of a pair of 4 m long APPLE type undulators. The low- and high-energy undulators will be installed side by side in a switch yard arrangement and will provide the highest possible photon flux within this photon energy range. Complete polarization control in both linear and circular modes will be available. Moreover, the envisioned quasiperiodic magnetic structure of the undulators will result in optimized suppression of the higher order harmonics. The optical design of the beamline is based on the Variable Line Spacing Plane Grating Monochromator (VLS PGM) design and will deliver 10^{12} - 10^{13} photons/second at the experimental stations with a resolving power higher than 10^4 over the full photon energy range. The theoretical performance of the beamline and the preliminary technical design of the undulators will be presented. The complications associated with the high heat load on the optical elements will also be addressed.

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Characterization of individual Fe₂O₃ coated carbon nanotube by scanning transmission X-ray microscopy

S Yang,^{1,3} J Wang,³ X Meng,¹ R Li,¹ X Sun,¹ TK Sham²

¹Department of Mechanical and Materials Engineering, The University of Western Ontario, London, Canada; ²Department of Chemistry, The University of Western Ontario, London, Canada; ³Canadian Light Source Inc., University of Saskatchewan, Saskatoon, Canada

Carbon Nanotubes (CNTs) have attracted tremendous attention due to their unique combination of mechanical, electronic and thermal properties. Recently, Fe₂O₃ nanoparticles, tubes and thin films, have also emerged due to their potential in many applications. A composite of these two nanostructured materials is of considerable interest and will enhance their future applications. Using ferrocene and oxygen as precursors, a thin layer of Fe₂O₃ nitrogen-doped CNTs (NCNTs) composite has been successfully prepared by the atomic layer deposition technique. The interaction between Fe₂O₃ and N-CNTs is important to their functionality and durability. Understanding such interaction in nanocomposites remains a challenge with conventional analytical techniques. While X-ray absorption near-edge structure (XANES) spectroscopy is powerful in determining the electronic structures of nanocomposites of a distribution of sizes, nanoscale chemical imaging of individual nanocomposite is most desirable. Scanning transmission X-ray microscopy (STXM) provides an excellent combination of capabilities of chemical speciation by XANES and nanoscale microscopy by zone plate optics. In this presentation, the STXM with a high spatial resolution of 30 nm at the SM beamline of the Canadian Light Source (CLS) has been used for the nanoscale chemical imaging and spectroscopy of a single Fe₂O₃ coated NCNT (Fe₂O₃/NCNT). XANES of the single Fe₂O₃/NCNT has been compared with that of NCNTs and Fe₂O₃. The results reveal that the chemical interaction between the Fe₂O₃ film and the NCNT substrate is very strong through charge redistribution, which is favourable for good adhesion and hence the stability of the composite for desired applications.

5P182

Effect of humidity on individual SnO₂ coated carbon nanotubes studied by in situ STXM

J Wang,¹ J Zhou,¹ H Fang,² TK Sham,³ C Karunakaran,¹ Y Lu,¹ G Cooper,⁴ AP Hitchcock⁴

¹Canadian Light Source Inc., University of Saskatchewan, Saskatoon, SK, Canada; ²School of Materials Science and Engineering, Harbin Institute of Technology, Harbin, Heilongjiang, China; ³Department of Chemistry, The University of Western Ontario, London, ON, Canada; ⁴BIMR, McMaster University, Hamilton, ON, Canada

Tin oxide (SnO₂) is an important functional material with many remarkable physical and chemical properties among which an important one is high receptivity variation in gases. Recently high-sensitivity humidity sensors based on a single SnO₂ nanowire have been demonstrated [1]. Applying SnO₂ as a coating on carbon nanotubes (CNT) significantly enhances the sensitivity to gases, and is being used as gas sensors [2]. *In situ* Scanning Transmission X-ray Microscopy (STXM) with humidity control at the 10ID-1 spectromicroscopy beamline at the Canadian Light Source was used to study the effect of humidity on SnO₂/CNT. 0.1 s X-ray absorption spectra of individual SnO₂ coated CNT were measured at various relative humidity (RH). At high humidity (RH=0.78), 10 to 30 nm of water is adsorbed on individual SnO₂/CNTs, demonstrating coating variation among individual CNTs. For some entangled SnO₂/CNT regions, as much as 100 nm condensed liquid water is detected, indicating strong interaction between SnO₂ and water.

1. Q. Kuang et al. *J. Am. Chem. Soc.* 129 (2007) 6070-6071.
2. Y.-L. Liu et al. *Thin Solid Films* 497 (2006) 355-360.

5P183

Microspectroscopic in-situ study of organic field-effect transistorsC Hub,¹ B Watts,² R Fink¹¹Univ. Erlangen-Nuremberg, Erlangen, Germany; ²Paul-Scherrer-Institut, SLS, Villigen, Switzerland

Ultrathin pentacene-based organic field-effect transistors (OFETs) on commercially available silicon nitride membranes suitable for transmission X-ray experiments were investigated. The devices produced by high-vacuum deposition show excellent electronic performance ($\mu = 0.6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, $I_{\text{on/off}} = 10^6$) comparable to state-of-the-art OFETs. STXM-experiments recorded with the PoLux-STXM at the SLS [1] correlate structural and electronic properties at highest spatial and spectral resolution. Local NEXAFS spectra were used to analyze the different orientations of the pentacene nanocrystals. We can prove that the NEXAFS contrast for individual microcrystals is due to azimuthal orientations of the crystallites. Since the overall thickness of the device is sufficiently thin, we can study the electronic properties of the device while it is operated. Spectral changes during OFET operation can, however, hardly be detected with the current setup. We discuss potential reasons of this finding. Most probably, the local excitations (core-excitonic states) are not sensitive enough to the polarized state when the gate voltage is switched on. In addition, the applicable currents affect only 10^{-2} of the molecules located at the interface to the dielectric. We acknowledge financial support from the BMBF (contract 05KS7WE1) and ICMM.

[1] J. Raabe, G. Tzvetkov, et al., Rev. Sci. Instrum. 79, 11370 (2008)

5P184

Spectroscopic imaging of the $[\text{Zn,Mg}]\text{O}/\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ interface using photoemission electron microscopyM Bär,¹ J P Theisen,² F Erfurth,² R G Wilks,¹ R Félix,¹ S Haas,¹ L Tati Bismaths,¹ F Reinert,² F Kronast,¹ L Weinhardt²¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany; ²Exp. Physik VII, Universität Würzburg, Würzburg, Germany

Thin-film solar cells based on a simple $n^+ \text{-ZnO}/i\text{-ZnO}/\text{CdS}/\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ structure reach efficiencies around 20%. Due to economic and ecological reasons, it would however be very attractive to sputter the ZnO window bilayer directly on the $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ "CIGSSe" absorber. However, only when using a $[\text{Zn,Mg}]\text{O}$ rather than $i\text{-ZnO}$ layer good solar cell efficiencies can be reached. Lab-based photoemission experiments recently revealed that due to sputter deposition of $[\text{Zn,Mg}]\text{O}$, Zn is incorporated into the CIGSSe absorber surface, resulting in a Zn-depleted window layer close to the interface and hence a rather complex chemical interface structure. Micro-spectroscopic investigations based on the combination of a tunable synchrotron light source with a photoemission electron microscope (PEEM) have emerged as a uniquely suited tool to study local electronic and chemical sample properties. We find that the collected PEEM images of a thin $[\text{Zn,Mg}]\text{O}$ layer deposited onto the CIGSSe are dominated by topography contrast caused by pronounced roughness of the polycrystalline absorber. Nevertheless, a significant lateral inhomogeneity of the Zn/Mg ratio can clearly be observed. Computing the Zn/Mg ratio from local Mg 2p and Zn 3d photoemission spectra from a series of energy filtered PEEM images (field of view: $10 \mu\text{m}$) confirms that observation. In our presentation, we will discuss our PEEM results also in relation to the resulting lateral variations of the electronic interface structure.

5P185

25 tesla pulsed-high-magnetic-field system for soft X-ray spectroscopyM Hayashi,¹ Y Narumi,¹ H Nojiri,¹ T Nakamura,² T Hirono,² T Kinoshita,² K Kodama,³ K Kindo⁴¹Institute for Materials Research, Tohoku University, Sendai, Japan; ²Spring-8/JASRI, Hyogo, Japan; ³Department of Mechanical Engineering, Nara National College of Technology, Nara, Japan; ⁴Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan

We have developed a 25 T pulsed high magnetic field system for soft X-ray spectroscopy. As the first application, we have measured soft X-ray magnetic circular dichroism (XMCD). In a conventional XMCD system, a magnetic field is provided by a superconducting magnet below 10 T and thus it has been used mostly for ferromagnetic compounds. Recently, XMCD of hard X-ray region using pulsed magnetic field up to 40 T has been succeeded [1] and the result shows the usefulness of high pulsed field XMCD. Combining soft X-ray and the pulsed magnetic field is much intensively desired because the energies of $2p\text{-}3d$ core absorptions of the $3d$ transition metals are in the soft X-ray region. We have assembled a new spectrometer by combining ultra-high vacuum and a large bore pulse magnet. As a power supply, we have developed a compact and portable capacitor bank storing 27.2 kJ of total energy with capacitance of 13.6 mF. Owing to the large capacitance, we can generate pulse field as long as 60 msec up to 25 T. The total electron yield method has been employed for recording absorption. The long pulse is of value to recording absorption by the total electron yield method because of the less electromagnetic induction noise. The power supply has various useful functions for XMCD measurement, such as automatic-charge-discharge, synchronization with polarization switching, and bipolar pulse current output. In this presentation, we will show the pulse magnetic system for soft X-ray MCD and some demonstrative results of soft X-ray MCD measurements under high magnetic field over 20T at BL25SU of SPring-8.

[1] Y. H. Matsuda *et al.*, Phys. Rev. Lett. **103** (2009) 046402

5P186

Study of OSEM with different subsets in grating-based X-ray differential phase-contrast imaging

K Zhang,¹ P Zhu,¹ Q Yuan,¹ W Huang,¹ X Liu,¹ Z Wu,² M Stampanoni,³ SA McDonald,³ F Marone³

¹Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China; ²University of Science and Technology of China, Hefei, China; ³Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland

The latest developments in X-ray imaging are associated with X-ray phase contrast computed tomography based on grating interferometry. Recently, a new "single-step" method is proposed to separate the phase information from other contributions by our team. Compared to the existing phase step approach this method can significantly reduce delivered dose and also simplify the data acquisition procedure. However, the image reconstruction procedures demand significant improvements of the traditional methods, and/or new algorithms have to be introduced to take advantage of the new "single-step" experimental method. In this letter, A fast iterative image reconstruction method-OSEM (Ordered Subsets Expectation Maximization) is applied in the new experiment technique, the effective range of OSEM parameters (such as iterative number, subset order) is verified. and the OSEM with various subset orders are studied by comparing their reconstructive image quality and convergent speed. Computer simulations and experimental results confirm the reliability of the OSEM algorithm in phase contrast computed tomography, which gives better images with higher spacial resolution and lower noise. We envisage that this development will also be of interest for potential future clinical applications.

5P188

Electron yield detection in scanning transmission X-ray microscopy: improving surface sensitivity

S Behyan,¹ B Haines,¹ C Karanukaran,² J Wang,² M Obst,² T Tyliczszak,³ SG Urquhart^{1,2,3}

¹Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada; ²Canadian Light Source, University of Saskatchewan, Saskatoon, SK, Canada; ³Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

We have modified a STXM at the Canadian Light source and the Advanced Light Source to be a surface sensitive technique, by using channeltron based total electron yield (TEY) detection mode which enables simultaneous bulk (transmission) and surface (TEY) measurements. The channeltron was mounted at the back of the sample, facing towards the surface of the sample in order to detect the secondary electrons ejected from the surface. This method provides for improved surface sensitive imaging of ultrathin films such as phase-separated Langmuir-Blodgett monolayer films, as well as differentiation of surface and bulk oxides of patterned metallic thin films. This contribution will outline the experimental challenges of this new method and the opportunities for correlative surface and bulk measurements of complex samples.

5P189

Young's interferometer at 90 eV with a versatile VUV apparatus

T Hatano,¹ S Ogasawara,¹ H Umetsu,¹ T Tsuru,¹ M Yamamoto¹

¹IMRAM, Tohoku University, Sendai, Japan

Interferometry is generally used in tests of precision optics. In VUV region, reflective optics coated with multilayer reflectors have a potential resolution of ten nm level. At-wavelength interferometry in a laboratory scale using a laser produced plasma (LPP) source would be a more versatile and convenient tool, while interferometry has been performed at synchrotron facilities for particular optics. We have developed a single vacuum chamber apparatus for versatile VUV experiments equipped with an LPP source. On a 900 mm × 1200 mm vacuum optical bench, various optics can be arranged. For experiments around 90 eV, a Mo/Si multilayer mirror and a Zr thin film are used as a bandpass filter. In the present study, Young's experiments were performed with an ordinary transmission double slit and a specially fabricated reflection double slit of both 80 μm separation. The LPP target was a W plate. The source size was estimated to be 50 μm from a pinhole camera image. It is small enough for a high spatial coherence over the double slit located at a distance of 800 mm from the source. A single slit and a collector optics were not used. Fringe patterns of 90 eV were successfully observed. The reflection double slit is composed of a Mo/Si multilayer reflector and a photoresist mask with an aperture of a double slit pattern. The period number of the multilayer is 30 in a selected part and 40 in the other part. The reflection phase difference between 30 and 40 period parts was evaluated to be 120° from the observed fringe shift.

5P190

Scanning transmission X-ray microscope at photon energies below 200 eV**T Tyliczszak¹**¹LBNL - Advanced Light Source, Berkeley, CA, United States

In last few years Scanning Transmission X-ray Microscopes (STXM) becomes valuable tool in many fields. At the Advanced Light Source, beamline 11.0.2, STXM branchline it is possible to illuminate the focusing zone plate with photons of energies down to 80 eV. However work below 200 eV requires special considerations. One of the difficulties is a relatively very short working distance, 70 to 180 micrometers. Another, even more significant problems are very high absorption in microscope optical elements (vacuum window, zone plate), requirements for thin samples and low detector efficiency. Regardless of those difficulties, spectro-microscopy of sulfur and potassium 2p absorption edges (130 eV – 170 eV) is a routine operation and yields many interesting scientific results¹. At present imaging at lower energies is possible, but obtaining spectral information is difficult. In this presentation current status and development to improve spectral information at absorption edges below 130 eV will be discussed. New, free standing zone plates will very likely make very low energy X-ray scanning microscopy with spectroscopic information possible.

1. K.L. Norlund, G. Southam, T. Tyliczszak, Y. Hu, Ch. Karunakaran, M. Obst, A. P. Hitchcock and L. A. Warren, Environ. Sci. Technol., 2009, 43 (23).

5P191

A rotatable photoelectron emission microscope combined with polarized synchrotron radiation**T Sekiguchi,¹ Y Baba,¹ I Shimoyama,¹ N Hirao,¹ A Narita,¹ M Md Abdul,¹ R Koswattage¹**¹Japan Atomic Energy Agency, Ibaraki, Japan

Recently, much thinner and higher-quality thin films are needed in the field of organic semiconductor and organic solar-cell development as next-generation devices. We report on the project started recently: Method to map direction of chemical -bonds in nanometer scale. We are striving to develop a unique instrument to measure polarization-angle dependence of Near-edge X-ray absorption fine structure (NEXAFS) spectra at nanometer level using photoelectron emission microscopy (PEEM), in order to understand creation and growth mechanisms of oriented domains. It is possible to measure XAFS spectra of microscopic regions magnified by the PEEM scope. The most unique point is the fact that the PEEM column can be rotated along the axis of synchrotron beam, so that one can measure polarization-angle dependences of such micro-XAFS spectra.

Moreover, we demonstrate that other experimental and theoretical methods which provide complementary information for chemical and electronic states of organic films. Such includes X-ray photoelectron spectroscopy (XPS), photon-stimulated ion desorption (PSID) spectroscopy, and molecular orbital calculation under equivalent core ($Z+1$) approximation. XPS allows chemical composition, chemical (charged) states, and thickness of the organic film. PSID sheds light on upwards/downwards direction of chemical groups, and interaction between adsorbed molecules and substrates. The $Z+1$ calculation gives comparably easier access to knowledge of nature of near-edge peaks.

5P192

Energy filtered photoelectron microscopy**K Winkler,¹ M Escher,² N Weber,² M Merkel,² B Kroemker¹**¹Omicron NanoTechnology, Taunusstein, Germany; ²FOCUS GmbH, Huenstetten, Germany

Photoelectron emission microscopy (PEEM) in combination with a high-resolution energy filter (E in the 100meV regime) is a non-destructive and versatile surface characterisation technique with the ability to solve upcoming scientific metrology issues. To identify the chemical compounds in a local sample area, energy-filtered PEEM is a very valuable metrology tool combining high spatial resolution with high-resolution spectroscopy. Continuous improvements of PEEM instruments nowadays enable local nano-spectroscopy with the highest lateral resolution in convenient laboratory conditions. Imaging XPS with unsurpassed lateral resolution and quantitative analysis of the local work function allow for a detailed understanding of the surface chemistry, including locally resolved doping effects on small structures used for semiconductor devices and even smaller silicon nano-wires. In addition, recent experiments have shown the feasibility for a new class of experiments for band structure analysis. Advanced spectroscopic PEEM instruments allow a new approach to analyse the electronic structures of samples. Thus band structure mapping with a large acceptance angle of $\pm 90^\circ$ without the need for eucentric sample rotation becomes possible. Together with full control over the analysed local area, the technique is ideally suited to investigate the electronic properties of single grains or small devices. Hence, this method opens up the path to a new class of experiments allowing e.g. dedicated local band structure tailoring. To identify potential device and materials technologies or to extend and compliment CMOS technology often requires a deep understanding of the basic materials science. In this field energy-filtered PEEM has established itself as a valuable surface metrology technique with numerous contributions to basic materials research. The PEEM technique has e.g. helped to better understand the preparation processes leading to microstructured crystallization. Today PEEM instruments play a key role in the growing field of plasmon and plasmon dynamics research. Moreover, the growing number of major scientific contributions have also helped to gain a deeper understanding of magnetic devices.

FRIDAY PROGRAM

6PL	VUVX Awards Session Chair: Chuck Fadley	timing includes 5 minute introduction & presentation for each award	8:40 - 10:35
LIFE SCIENCES INSTITUTE 2			
6PL1	Uwe Hergenbahn 8:40 Photoionization and autoionization of weakly bonded clusters	VUVX Conference Award in atomic, molecular and optical physics	
6PL2	Eli Rotenberg 9:25 Observation of composite particles in graphene by ARPES	VUVX Conference Award in condensed matter physics	
6PL3	Suet Yi Liu 10:10 Time-resolved photoelectron imaging using a femtosecond UV laser and a VUV free electron laser	VUVX Student Award	
Coffee			10:35 - 11:00
6A	Clusters Chair: Edwige Otero	11:00 - 12:30	
LIFE SCIENCES INSTITUTE 2			
6A1	Matthias Neeb (invited) 11:00 XMCD spectroscopy on mass-selected transition metal clusters using a Penning ion trap		
6A2	Shojun Hino 11:30 The electronic structure of multiple atoms entrapped in endohedral fullerenes		
6A3	Minna Patanen 11:50 Direct experimental determination of atom - molecule - solid binding energy shifts for Sb and Bi		
6A4	Masanari Nagasaka 12:10 Structural changes of small Kr-Xe mixed clusters with different compositions studied by soft X-ray photoelectron spectroscopy		
6B	Graphene and other carbon materials Chair: Eli Rotenberg	11:00 - 12:30	
FOREST SCIENCES 1005			
6B1	Claire Berger (invited) 11:00 Epitaxial graphene as a nearly ideal graphene band structure system		
6B2	Ebrihim Najafi 11:30 Polarization dependence of the C 1s X-ray absorption spectra of carbon nanotubes		
6B3	Osamu Endo 11:50 Orientation of n-Alkane in thin films on graphite (0001) studied by C K-NEXAFS		
6B4	Emanuele Pace 12:10 Diamond photodetectors for X-ray absorption spectroscopy applications		
Lunch [NOTE SHORTER THAN PREVIOUS DAYS]			12:30 - 13:30
6C	Dynamics (2) Chair: Uwe Becker	13:30 - 15:10	
LIFE SCIENCES INSTITUTE 2			
6C1	Majed Chergui (invited) 13:30 Probing ultrafast molecular dynamics in solutions from the UV to the hard X-ray range		
6C2	Tae Kyu Kim 14:00 Probing electronic dynamics in solvated transition metal complexes by femtosecond soft X-ray spectroscopy		
6C3	Anthony Dutoi 14:30 Tracing molecular electronic excitation dynamics in real time and space		
6C4	Wojciech Gawelda 14:50 Ultrafast X-ray spectroscopies with current and future light sources		
6D	X-ray scattering Chair: Donglai Feng	13:30 - 15:10	
FOREST SCIENCES 1005			
6D1	Beatriz Roldán Cuenya (invited) 13:30 Atomic vibrations in metal nanostructures		
6D2	Sebastian Brück 14:00 Unraveling the magnetic depth profile of a buried ferromagnet/antiferromagnet interface: A soft X-ray resonant magnetic reflectometry study of Fe/MnPd		
6D3	Robert Gordon 14:30 Studying low-energy core-valence transitions with bulk sensitivity using q-dependent NIXS		
6D4	Pieter Glatzel 14:50 Resonant inelastic hard X-ray scattering in chemical research		
6PL4	CLOSING CEREMONY Chair: Stephen Urquhart		15:10 - 15:30
LIFE SCIENCES INSTITUTE 2			

6PL1

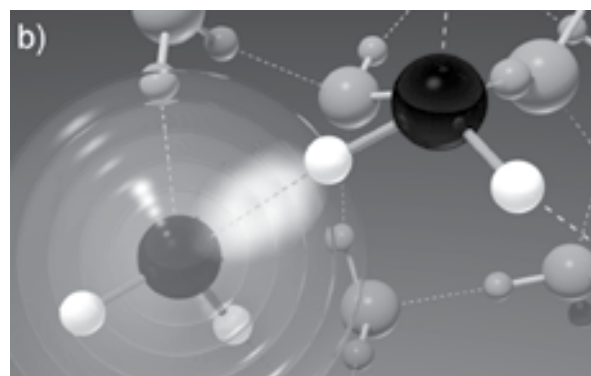
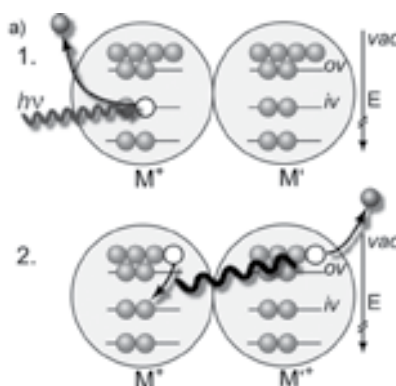
Photoionization and autoionization of weakly bonded clusters

Uwe Hergenhahn¹¹ Max-Planck-Institut für Plasmaphysik, EURATOM Association, 85748 Garching, Germany

Using clusters as nano-laboratories we can study the influence of aggregation on the electronic structure for weakly bonded systems. Examples are given by hydrogen-bridge bonded clusters, such as water clusters, and clusters which form due to van-der-Waals interactions, e.g. from noble gases. Photoionization allows to compare the electronic structure of these entities to the respective monomers. In my presentation I will give some examples from our work with electron spectroscopy on free cluster jets from a supersonic beam expansion, using synchrotron radiation from the storage ring BESSY II (Berlin, Germany).

A lowering of the double-ionization potential in clusters compared to the isolated monomer has long been known. Autoionization channels in clusters may therefore open, which are energetically unfeasible without the cluster environment. For the case of weakly bonded clusters, the decay into these cluster specific channels is now discussed as 'Intermolecular/Interatomic Coulombic Decay' (ICD). Characteristic for ICD is a final state, in which two charges are distributed at two neighbouring sites in a cluster. I will describe experiments in which electrons emitted due to autoionization by ICD have been directly detected, e.g. in water clusters. Detecting both electrons in coincidence turned out to be a powerful technique to isolate a signature of ICD. This phenomenon is expected to be universal, and may have important applications e.g. for investigating the chemistry of solutions, and for radiation biology.

Schematic of Inter-molecular Coulombic Decay in water clusters [a, step 1: photoionization, step 2: ICD] and an artist's impression of the energy transfer within a cluster [b].



Uwe Hergenhahn received his Diplomarbeit from the Technical University of Berlin in 1991, and his PhD under the supervision of Uwe Becker and Ulrich Heinzmann on spin polarization of Auger electrons in 1996. From 1996 to 1999 he was a postdoctoral fellow at the Fritz-Haber Institute (Berlin) working mainly at NSLS on inner shell photoionization of molecules. In 2000 Dr. Hergenhahn became staff scientist at the Max-Planck-Institut für Plasma Physics (Garching, Germany), although he has remained based in Berlin. In 2004, he spent an extended period as Visiting Research Professor in the Ueda group at Tohoku University, Sendai (Japan). In 2005, Dr. Hergenhahn completed his habilitation. To date Uwe has worked on

numerous synchrotron radiation sources (BESSY, ESRF, NSLS, SPring8, Hasylab and at the Free Electron Laser FLASH) in the VUV as well as in the X-ray range. He has made outstanding contributions in fundamental understanding of the physics of inner-shell excitation and decay phenomena. His research deals with electronic structure and the relaxation of excited states and in clusters and molecules, and with coherence in electronic transitions and electron beams.

VUVX CONFERENCE AWARD IN ATOMIC, MOLECULAR AND OPTICAL PHYSICS

"For creativity in demonstrating new phenomena of general interest in atomic and molecular physics, including intermolecular coulombic decay in molecules and clusters, complete photoelectron and Auger measurements with spin resolution and resonant decay, asymmetry in photoionization of chiral molecules, and vibrational excitation with inner-shell excitations"

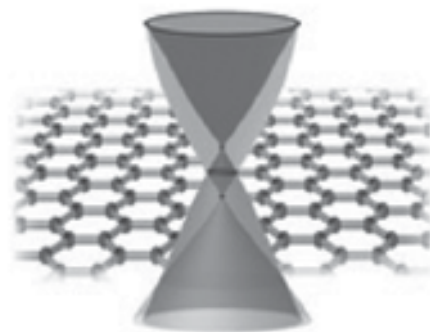
6PL2

Observation of composite particles in graphene by ARPES

Eli Rotenberg¹¹Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, Berkeley, CA, United States.

The lifetime of electrons and holes in doped graphene is important both as a practical matter for new devices as well as to answer fundamental questions about the many-body interactions among graphene's effectively massless carriers. Here we report angle-resolved photoemission measurements of quasi-freestanding graphene and show that the well-known conical, linear bands crossing at the Dirac energy do not represent the actual excitation spectrum of doped graphene. In reality, the spectrum is split into two components, consisting of an ordinary quasiparticle band, and a dispersing "plasmaronic" band consisting of a core hole bound to a plasmon. As a result, the single Dirac crossing of the valence and conduction bands is replaced by 3 Dirac crossings: between ordinary holes, between one hole and one plasmaronic band, and between plasmaronic bands.

The energy bands of complex particles known as plasmarons have been seen for the first time by an international team of scientists working with graphene at the Advanced Light Source, led by Aaron Bostwick and Eli Rotenberg. The discovery leads to a new picture of graphene's already-bizarre electronic properties and may hasten the day when these crystalline sheets of carbon, just one atom thick, can be used to build ultrafast computers and other electronic, photonic, and plasmonic devices on the nanoscale



Eli Rotenberg received his B.Sc. in Applied and Engineering Physics from Cornell University in 1987. He did graduate studies in Physics at Berkeley, studying core level spectroscopy with Marjorie Olmstead, receiving his PhD in 1993. Dr. Rotenberg continued as a postdoc with Prof. Steve Kevan (U. Oregon), working at the Advanced Light Source. During this time he developed an instrument for Angular Resolved PhotoElectron Spectroscopy (ARPES), together with Jonathan Denlinger and Brian Tonner. Dr. Rotenberg was employed as an ALS staff scientist in 1996, where he continued to develop ARPES instrumentation and his scientific program. He is a fellow of the American Physical Society (2008). He received the Peter Mark Memorial Award of the

American Vacuum Society in 2001, for "furthering our knowledge of nanophase and reduced dimensionality systems by creative use of angle-resolved photoemission" and the 2009 Kai Siegbahn prize for "the creation of the ARPES 'Electronic Structure Factory' endstation at the ALS and for his outstanding scientific work in electron spectroscopy".

VUVX CONFERENCE AWARD IN CONDENSED MATTER PHYSICS

"For his development of an advanced soft X-ray angle-resolved soft photoemission facility, and its insightful application to a broad variety of forefront problems in surface and condensed matter physics, including magnetic multilayer structures, surface states, reduced dimensionality materials, strongly correlated materials and superconductors, photoelectron diffraction and holography, and most recently graphene"

6PL3

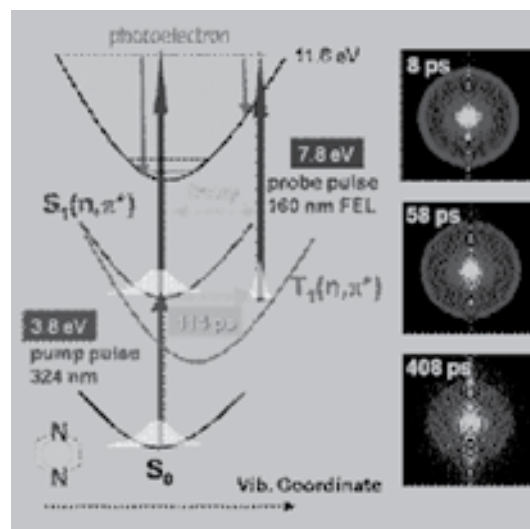
Time-resolved photoelectron imaging using a femtosecond UV laser and a VUV free-electron laser

Suet Yi Liu^{1,2}, Y. Ogi¹, Fuji¹, K. Nishizawa^{1,2}, T. Horio³, T. Mizuno¹, H. Kohguchi^{1,4}, M. Nagasono⁵, T. Togashi^{5,6}, K. Tono⁵, M. Ybashi⁵, Y. Senba⁶, H. Ohashi^{5,6}, H. Kimura^{5,6}, T. Ishikawa⁵, T. Suzuki^{1,2,3}

¹ RIKEN, Wako, Japan. ² National Chiao Tung Univ., Hsinchu, Taiwan. ³ Kyoto Univ., Kyoto, Japan. ⁴ Hiroshima Univ., Higashi-Hiroshima, Japan. ⁵ RIKEN XFEL, Sayo, Japan. ⁶ Japan Synchrotron Radiation Research Inst., Sayo, Japan.

The first time-resolved photoelectron imaging (TR-PEI) using a femtosecond tunable UV laser and VUV free electron laser (SCSS) constructed at SPring-8 in Japan is presented. Pyrazine (C₄H₄N₂: 1,4-diazabenzene) in a supersonic molecular beam was excited to the first (S₁) or second (S₂) excited singlet state by a femtosecond pump laser pulse at 324 or 260 nm, respectively, and subsequent ultrafast electronic dynamics were interrogated by photoelectron spectroscopy using the FEL probe pulse at 161 nm. The photoelectron speed and angular distributions were visualized by two-dimensional photoelectron imaging apparatus that was optimized for VUV experiment through the test experiments using He(I) light source in the laboratory. With the UV pump and VUV probe technique, ultrafast S₁-T₁ intersystem crossing and S₁-S₀ internal conversion in pyrazine in a supersonic molecular beam were clearly observed in the time profiles of photoelectron intensity and photoelectron images. The VUV radiation allowed us to observe the entire Franck-Condon envelope in photoionization from a transient electronic state, which was not possible in UV-UV experiment in the laboratory. Our study clearly demonstrates the exciting opportunities of picosecond TR-PEI experiment on photoinduced chemical dynamics of large polyatomic molecules with a SASE FEL and a tunable UV femtosecond laser.

(left) Dynamics scheme of 324 nm pump + 161 nm probe. (right) Photoelectron images observed at pump-probe time delays of 8, 58 and 408 ps.



Suet Yi (Shirley) Liu received her B.Sc. in Chemistry from National Tsing Hua University (NTHU), Hsinchu, Taiwan in 2004, and her MSc. in chemistry from NTHU in 2006. She is presently carrying out her PhD studies, under co-supervision of Yuan-Pern Lee (NTHU) and Toshinori Suzuki (Kyoto University & Riken). Her PhD studies have involved development of both lab-laser and FEL based time resolved photoelectron imaging as a probe of molecular photoionization dynamics. She expects to graduate in Dec 2010.

VUVX STUDENT PRIZE

"For her creative work in molecular physics involving the development of a first instrument for carrying out time-resolved photoelectron energy and angle imaging by a femtosecond UV laser and a VUV free-electron laser. Her research has included extensive instrumentation design, as well as data analysis"

6A1 (Invited)**XMCD spectroscopy on mass-selected transition metal clusters using a Penning ion trap**

M Neeb,¹ S Peredkov,¹ S Peters,¹ W Eberhardt,¹ H Kampschulte,² J Meyer,² B Hofferberth,² F Menges,² G Niedner-Schatteburg²

¹Helmholtz-Zentrum-Berlin, Wilhelm-Conrad-Röntgen Campus Adlershof (BESSYII), Berlin, Germany; ²Technische Universität Kaiserslautern, Fachbereich Chemie, Kaiserslautern, Germany

An experimental setup has been installed at the BESSY II storage ring which is intended to record X-ray absorption spectra of free mass-selected clusters using bright soft X-ray radiation. The goal of the unique setup is to provide XMCD spectra of mass-selected cluster ions using circularly polarized X-ray radiation. For this a Fourier-Transform-Ion-Cyclotron-Resonance mass spectrometer (FT-ICR) has been installed which provides a strong axial magnetic field for ion trapping. The photoabsorption signal is obtained by recording the fragmentation pattern produced after X-ray absorption and subsequent Auger decay of the core-excited parent cluster ion. The experimental setup and first X-ray absorption spectra will be discussed. Furthermore, upon collisional cooling of small Co clusters a clear dichroic signal is observed when circular polarisation is used.

6A2**The electronic structure of multiple atoms entrapped in endohedral fullerenes**

S Hino¹

¹Ehime University, Matsuyama, Ehime, Japan

The electronic structure of endohedral fullerenes depends on the carbon cage size, symmetry of the carbon cage, the entrapped species, the oxidation state of the entrapped species and so on. We have been measuring the ultraviolet photoelectron spectra of both empty and endohedral fullerenes and found that principally the cage symmetry and the oxidation state of entrapped species dominated the electronic structure of mono metal atom entrapped endohedral fullerenes of the same numbered carbon atoms (empirical rule). It was found that this rule could not be applicable to $\text{Ti}_2\text{C}_2@\text{C}_{78}$ and $\text{La}_2@\text{C}_{78}$, but applicable to $\text{M}_2@\text{C}_{82}$ (M=Y, Lu, Er), $\text{M}_2\text{C}_2@\text{C}_{82}$ (M=Ti, Y, Lu, Er). We will present ultraviolet photoelectron spectra of $\text{Sc}_3\text{N}@\text{C}_{78}$, $\text{La}_2@\text{C}_{80}$, $\text{Ce}_2@\text{C}_{80}$, $\text{Lu}_2@\text{C}_{80}$ and $\text{Lu}_2\text{C}_2@\text{C}_{80}$, and discuss whether the empirical rule holds in these endohedral fullerenes. We also present theoretical calculation of some of these fullerenes and discuss the oxidation state and geometry of the entrapped species.

6A3

Direct experimental determination of atom — molecule — solid binding energy shifts for Sb and Bi

M Patanen,¹ S Aksela,¹ S Urpelainen,¹ H Aksela¹

¹Department of Physics, University of Oulu, Oulu, Finland

Binding energy [BE] shifts of core levels between atoms, molecules and their solid samples are fundamental data for different branches of electron spectroscopy and the theory of the electronic structures of the molecules, clusters, and solids. The accurate atom-solid BEs and their shifts are useful reference values in the experimental studies of clusters. The experimental atom-solid BE shifts are, however, not very accurately known, because for free atoms and molecules BE values are measured with respect to vacuum level whereas the solid state values are measured with respect to the Fermi level. In order to bring the values to the common energy scale solid state values should be corrected by the work function of the sample, which is rather difficult to measure accurately, and it is desirable to obtain shift values directly from one single experiment. We have used a simple method in order to observe both vapor and solid state spectra with identical experimental conditions. A cool needle is located into the vapor beam and spectra from the vapor around the tip and from the solid layer condensed on the tip are simultaneously observed. The surface of the tip is covered by the sample's work function potential and the vapor atoms are in this potential in the vicinity of the surface. The spectra have the same reference energy level and no work function correction is needed. In this study, we have measured the Bi 4*f* and Sb 4*d* photoelectron spectra [PES] using this method. These samples are especially interesting because they evaporate as molecular species which can be fragmented further pyrolytically using a special inductively heated oven system. This provides an interesting possibility to experimentally determine the atom-molecule-solid shifts.

6A4

Structural changes of small Kr-Xe mixed clusters with different compositions studied by soft X-ray photoelectron spectroscopy

M Nagasaka,¹ N Kosugi,¹ E Ruehl²

¹Institute for Molecular Science, Okazaki, Japan; ²Physikalische Chemie, Freie Universitaet Berlin, Berlin, Germany

Heterogeneous clusters consisting of different atoms show a rich structural behavior with changing the mixing ratio. Theoretical works suggest that the structures of the mixed clusters are dependent on competition of several factors, such as atomic radii, surface energies, and interaction energies between different molecules. But there exist only a few experiments on the structures of small mixed clusters. Recently, we have measured X-ray photoelectron spectroscopy [XPS] of small Kr₃₀ clusters and observed different binding energy shifts dependent on the surface sites.

[1]. In this work, we have studied the structures of small Kr-Xe mixed clusters at different compositions by using XPS in the Xe 4*d*_{5/2} and Kr 3*d*_{5/2} regimes. The experiments were performed at the soft X-ray undulator beamline BL3U of UVSOR-II. The Kr-Xe mixed clusters were formed by a supersonic expansion of the primary gas mixtures containing Xe between 1 – 5 %. Systematic binding energy shifts and the intensity changes in XPS are observed with the structural changes of the mixed clusters. These changes are evidenced from calculations of the binding energy shifts taking into account induced dipole interactions. As a results, we estimate that a small Xe core is embedded on the surface of the Kr cluster in a Xe₅Kr₂₇ cluster. Two Xe cores are expected in a Xe₁₁Kr₂₆ clusters. The Xe cores are growing with increasing Xe content on the surface and merge in a Xe₁₄Kr₂₂ cluster. Finally separated layers between the Xe and Kr clusters are formed in a Xe₂₂Kr₁₄ clusters.

[1] T. Hatsui *et al.* J. Chem. Phys. **123**, 154304 [2005].

6B1 (Invited)**Epitaxial graphene as a nearly ideal graphene band structure system**

C Berger^{1,2}, M Sprinkle,¹ J Hicks,¹ X Wu,¹ M Ruan,¹ Y Hu,¹ M Potemski,² P Soukiassian,³ A Tejada,^{2,4} A Taleb-Ibrahimi,⁴
E H Conrad,¹ W A de Heer¹

¹Georgia Institute of Technology, Atlanta, United States; ²CNRS, Grenoble, France; ³Université Paris-Sud, Orsay, France; ⁴Synchrotron SOLEIL, Saint-Aubin, France

Multilayered epitaxial graphene on SiC is a new material composed of one up to about a hundred rotationally stacked graphene layers. This original non-graphitic commensurate rotated stacking preserves the integrity of the band structure of the graphene layers (massless Dirac particles), as if the layers were effectively decoupled. This is experimentally demonstrated on cm² size multilayered graphene sheets grown by thermal decomposition of the 4H-SiC (000-1) surface in a controlled environment induction furnace. Ripple-less atomically flat surfaces over several tens of microns are observed by AFM and STM. The graphene layers drape continuously over the SiC steps. Angle-resolved photoemission experiments show a set of linearly dispersing bands (Dirac cones) at the graphene K point. Each cone corresponds to an individual macroscale graphene sheet in a multilayer stack, where AB-stacked sheets can be considered as low density faults. The deviation from linearity observed for single layers grown on the SiC (0001) face is not observed here. The graphene-like band structure is also observed in the spectroscopic response in magnetic field (IR magneto-spectroscopy and scanning tunneling spectroscopy), where the Landau levels show the graphene characteristic dispersion. Transport and spectroscopic measurements indicate high mobility, up to 250,000 cm²/Vs at room temperature. Epitaxial graphene can be patterned using standard lithography methods to define top and side-gated high mobility devices. Thousands of transistors have been produced on a single mm² size chip demonstrating the strong potential of multilayered epitaxial graphene for carbon-based electronics.

6B2**Polarization dependence of the C 1s X-ray absorption spectra of carbon nanotubes**

E Najafi¹, A Hitchcock,¹ J Guan,¹ S Denomme,¹ B Simard¹

¹Brockhouse Institute for Materials Research, McMaster University, Hamilton/ON, Canada; ²Steele Institute for Molecular Sciences, National Research Council of Canada, Ottawa/ON, Canada; ³Canadian Light Source Inc, University of Saskatchewan, Saskatoon/SK, Canada

The surface chemistry and structural defects of carbon nanotubes (CNT) is of fundamental importance for their applications in various electronic and mechanical applications [1]. We are developing C 1s near-edge X-ray absorption fine structure (NEXAFS) spectromicroscopy in a scanning transmission X-ray microscope (STXM) as a probe the structure of individual CNT. In multi-walled CNT with low defects, the π^* peak (285 eV) has a strong dichroic response with almost zero intensity when the E-vector is parallel to the long axis of high quality tubes [2]. High quality single-walled CNT have a reduced but still significant π^* dichroism [3]. However the π^* dichroism is much lower in CNT produced with methods such as CVD where structural order is lower. The dichroism is absent when the tube is amorphized by ion or electron beam bombardment. Given sufficient data quality, the distribution of defects can be visualized and quantitatively mapped along CNT. We are exploring how C 1s dichroism of individual CNT can assist development of CNT-based devices which require specific defect properties e.g. defect-free or with a controlled, periodic defect density.

1. Baughman, et al *Science* **2002**, 297, 787. 2. Najafi, E et al, *A. Small* **2008**, 4,12, 2279. 3. Najafi, E. et al, *J. Am. Chem. Soc.* (in review)

6B3

Orientation of *n*-alkane in thin films on graphite (0001) studied by C K-NEXAFS

O Endo,¹ R Sumii,² K Amemiya,² M Nakamura,³ N Kosugi,⁴ H Ozaki¹

¹Department of Organic and Polymer Materials Chemistry, Faculty of Engineering, Tokyo University of Agriculture and Technology, Tokyo, Japan; ²KEK-PF, Tsukuba, Japan; ³Department of Applied Chemistry and Biotechnology, Faculty of Engineering, Chiba University, Chiba, Japan; ⁴UVSOR, Institute for Molecular Science, Okazaki, Japan

The thin film growth of *n*-alkane on inert solid surfaces including graphite (0001) under UHV is of importance for clarifying the property of alkyl chains in a condensed phase. The *n*-alkane in the first layer physisorbed on graphite form lamellae with their chain axes parallel to the surface. The orientation of the carbon skeleton is, however, controversial between parallel (flat-on) and perpendicular (edge-on) to the surface. Moreover, the structures of a multilayer grown on the lamellae have not been studied well. In this study, we have measured the C K-NEXAFS spectra of the *n*-C₁₂H₂₆ (C12) films on graphite (0001). In the normal incidence spectra, the 1s → σ_{CH}^*/R resonance of the *n*-alkane was distinguished at a lower energy than the absorption edge of the substrate. The *ab-initio* calculations carried out by the GSCF3 code for an isolated *n*-butane suggest that the σ_{CH}^*/R resonances parallel and perpendicular to the carbon skeleton exist at 288.7 eV and 289.3 eV, respectively. The resonances are merged into weak one directed along the CH bond ($\sigma_{\text{CH}}^*/R_{\text{CH}}$) at 288.8 eV upon the adsorption with the flat-on orientation on the graphite surface represented by a small grapheme-like molecule. In the experimental spectra, the $\sigma_{\text{CH}}^*/R_{\text{CH}}$ resonance was observed at 286.8 eV for the C12 first layer on graphite. As the film thickness increases, another peak assigned to the σ_{CH}^*/R (perpendicular) resonance grows at 287.8 eV. These spectral features are attributed to the flat-on orientation of the C12 molecules in the first layer, and the increase of the molecules with the edge-on orientation in a multilayered film.

6B4

Diamond photodetectors for X-ray absorption spectroscopy applications

E Pace,^{1,2} A De Sio,^{1,2} Z Pan,³ Z Wu,³ Y Huang,⁴ Z Jiang,⁴ F D'Acapito,⁵ A Marcelli⁶

¹Dip. di Fisica e Astronomia, Università di Firenze, Firenze, Italy; ²INFN, Sezione di Firenze, Firenze, Italy; ³National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, China; ⁴Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai, China; ⁵CNR-INFM-OGG, ESRF, GILDA, Grenoble, France; ⁶INFN - Laboratori Nazionali di Frascati, Roma, Italy

Synchrotron radiation (SR) is a fundamental tool for X-ray research. In particular, X-ray absorption spectroscopy (XAS) accesses information as electronic properties, local structure or chemical-physical state in condensed-matter studies. Ionization chambers (ICs) are the most widely used XAS detectors for transmission measurements because of their reliability, high linearity and good stability. Recently, solid-state detectors have been considered and Si p-i-n has been applied to high fluxes (10¹¹ ph/s), where the linearity of ICs is no longer guaranteed. Silicon photodiodes exhibit an extremely linear response in at least 5 decades but show diffraction peaks. Diamond is an ideal substrate to produce radiation-hard, low dark current (< 1 pA/cm²), visible-blind and fast-response X-ray detectors with a high S/N ratio. Diamond detectors were tested as SR monitor capable to withstand the high photon flux density of the 3rd generation SR sources. Being the lowest X-ray-absorbing solid-state dielectric material, diamond maximizes the flux through thin self-standing devices with minimal spectral effect down to the soft X-ray range. We will present results of X-ray tests of photoconductors based on different diamond substrates performed at NSRL and SSRF in China and at GILDA, ESRF in France. The results will be compared to standard ICs for XAS applications in terms of spectral quality, noise and linearity in the 4-50 keV energy range.

6C1 (Invited)**Probing ultrafast molecular dynamics in solutions from the UV to the hard X-ray range****M Chergui**¹¹Ecole Polytechnique Fédérale de Lausanne, Lab. of Ultrafast Spectroscopy, Lausanne, Switzerland

By combining various ultrafast laser techniques with ps and fs X-ray absorption spectroscopy, we can fully identify the photocycle of solvated species. We will review some of our recent results on the solvation shell changes around atomic solutes, on the dynamics of binuclear molecular complexes, and on the structural changes induced by electron transfer and spin changes in metal-based molecular complexes.

6C2**Probing electronic dynamics in solvated transition metal complexes by femtosecond soft X-ray spectroscopy****N Huse,**¹ **H Cho,**^{1,2} **T K Kim,**² **L Jamula,**³ **J K McCusker,**³ **F M F de Groot,**⁴ **R W Schoenlein**^{1,5}¹Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States; ²Department of Chemistry, Pusan National University, Busan, Republic of Korea; ³Department of Chemistry, Michigan State University, East Lansing, MI, United States;⁴Department of Chemistry, Utrecht University, CA Utrecht, Netherlands; ⁵Material Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

The knowledge of temporally varying valence electronic structures during ultrafast processes is vital in understanding the rearrangement of chemical bonds and their cooperative relationship with atomic position. For this purpose, ultrafast soft X-ray absorption spectroscopy of first-row transition metal complex at metal L-edges is appropriate for delivering detailed information on the evolution of electronic structure. Herein we report femtosecond soft X-ray spectroscopy of solvated Fe(II) complex for the first time. Our data provide detailed information on the changes of metal-ligand interactions upon photo-induced metal-to-ligand charge transfer that are accompanied by spin-state conversion and a dilation of the ligand cage. The results of this work demonstrate the feasibility and potential of femtosecond soft X-ray absorption spectroscopy to study ultrafast processes in liquid phase by probing dynamic changes of valence electron orbitals.

6C3

Tracing molecular electronic excitation dynamics in real time and space

A D Dutoi,¹ L S Cederbaum,¹ M Wormit,² A Dreuw²

¹Theoretische Chemie, Heidelberg, Germany; ²Physikalische und Theoretische Chemie, Frankfurt, Germany

Understanding energy transfer after excitation has enormous relevance to biological processes, such as photosynthesis, as well as being of purely fundamental interest. We present a method for studying the movement of electrons and energy within and between electronically excited molecules. The dynamically changing state is a many-electron wavepacket. We have developed the tools necessary for following the separate motions of the particles and holes. In addition to demonstrating our propagation and analysis machinery, the results show a dramatic difference in excitation-energy transfer rates in a neon chain as a consequence of initial polarization. Furthermore, already in a system with three constituents, an important aspect of multiple coupled systems appears, in that one absorbing system essentially shields another, changing the effective site-wise coupling parameters. Finally we show interesting examples where an initially local excitation results in a charge separated state, because the excited electron and the vacant hole have different mobilities through different regions of the molecule.

6C4

Ultrafast X-ray spectroscopies with current and future light sources

W Gawelda,¹ A Galler,¹ R Abela,² C Bressler¹

¹European XFEL GmbH, Hamburg, Germany; ²SwissFEL Project, Paul-Scherrer Institut, Villigen-PSI, Switzerland

X-ray spectroscopic tools, such as EXAFS and XANES, allow measuring local geometric and electronic structure of molecular systems, even in disordered media. X-ray emission spectroscopy delivers direct information about the electronic spin state. Implementing these tools in ultrafast experiments at present synchrotron light sources permits to record a complete molecular movie of an ongoing chemical reaction, which includes the elementary steps in light-driven processes. We have used ps-resolved XANES and EXAFS to monitor geometrical structure changes of the molecule after the spin transition is complete, while fs XANES was measured to observe the evolution of this process in real-time. Finally, a recent experiment exploiting ps-XES of the K-alpha emission established a direct measurement of the short-lived (0.7 ns) high-spin state. The extension of these spectroscopic techniques using fs X-ray pulses derived from X-ray Free Electron Lasers will allow us to deliver a complete dynamical description of the interplay between nuclear, electronic and spin degrees of freedom. Present status of the experiments will be discussed as well as a short outlook towards the design of a scientific instrument Femtosecond X-ray Experiments (FXE) planned at the European XFEL will be given.

6D1 (Invited)

Atomic vibrations in metal nanostructures

B Roldán Cuenya¹¹Department of Physics, University of Central Florida, Orlando, FL, United States

Metallic nanostructures are of great interest in many scientific fields due to their novel size-dependent physical and chemical properties. Intriguing effects such as phonon confinement and phonon localization at interfaces have been observed on low dimensional systems. Such modifications in the vibrational (phonon) density of states (PDOS) of nanoscale materials are of scientific and technological relevance, because they profoundly affect their thermodynamic properties. To study these effects homogeneous and size-selected nanostructures are needed. We have synthesized size- and shape-selected ^{57}Fe , $^{57}\text{Fe}_x\text{Pt}_{1-x}$, and $^{57}\text{Fe}_x\text{Au}_{1-x}$ nanoclusters (NCs) with well defined interparticle distances by means of diblock copolymer encapsulation. The clusters were supported on $\text{TiO}_2(110)$ and $\text{SiO}_2/\text{Si}(111)$. The size- and composition-dependent vibrational dynamics of these clusters was measured by nuclear resonant inelastic X-ray scattering (NRIXS). An enhancement of the density of low- and high-energy phonon modes as well as non-Debye-like behavior was observed on ^{57}Fe clusters. The latter effects were found to depend on the chemical nature of the surface shell on the NCs. Drastic deviations were observed in the PDOS of $^{57}\text{Fe}_x\text{Au}_{1-x}$ and $^{57}\text{Fe}_x\text{Pt}_{1-x}$ NCs with respect to the PDOS of their respective bulk alloys. The PDOS of fcc $^{57}\text{Fe}_{0.75}\text{Pt}_{0.25}$ [core]/PtSi(shell) NCs was found to retain features of bulk ordered Fe_3Pt Invar alloys, in particular the transverse-acoustic $[110] \text{TA}_1$ mode near 9 meV. Apparently, this mode is not affected by size effects and its presence is a pre-requisite for the persistence of Invar-related effects in Fe_3Pt NCs.

6D2

Unraveling the magnetic depth profile of a buried ferromagnet/antiferromagnet interface: a soft X-ray resonant magnetic reflectometry study of Fe/MnPd

S Brück,^{1,2} S Macke,² X Ji,³ Q Zhan,³ E Goering,² K M Krishnan³¹Faculty of Physics, University of Würzburg, Würzburg, Germany; ²Max Planck Institute for Metals Research, Stuttgart, Germany;³Dept. of Materials Science and Engineering, University of Washington, Seattle, Washington, United States

Non-destructive, deep probing X-ray techniques especially the so called soft X-ray resonant magnetic reflectivity (XRMR) are a new promising approach to tackle the problem of magnetism at buried interfaces. Using X-ray magnetic circular dichroism (XMCD) as a contrast mechanism in X-ray reflectivity, XRMR ultimately provides element-selective magnetic and chemical depth profiles of layered samples. We investigate a bilayer exchange-bias system composed of Fe/MnPd using XMCD and XRMR. The absorption and XMCD data at the Fe L and Mn L edges are used to derive the optical and magneto-optical properties of the individual layers. Then the structural and magnetic depth profiles of the sample are obtained from XRMR. From reflectivity measurements at the Fe L and Mn L edges, a precise magnetic depth profiling of the interface region between the ferromagnet (F) and antiferromagnet (AF) is carried out. It reveals rotatable and pinned uncompensated Mn moments in the AF [1]. By comparing the signs and magnitudes of the absorption, the relative coupling directions of all three kinds of moments, Fe and pinned and rotatable Mn, in the system are determined [2].

[1] S. Brück et al. *Phys. Rev. Lett.* **101**, 126402 (2008).[2] S. Brück et al. *Phys. Rev. B* **81**, 134414 (2010).

6D3

Studying low-energy core-valence transitions with bulk sensitivity using q -dependent NIXS

R A Gordon,^{1,2} G T Seidler,² T T Fister,³ K P Nagle²

¹Dept. of Physics, Simon Fraser University, Burnaby, BC, Canada; ²Dept. of Physics, University of Washington, Seattle, WA, United States; ³Chemical Sciences and Engineering, Argonne National Laboratory, Argonne, IL, United States

Absorption-based studies of low-energy atomic edges possess an inherent challenge in distinguishing surface and bulk contributions to the measured signal. The nature of the absorption process itself, being predominantly dipole in character, can also be a limiting factor in understanding electronic structure, particularly for correlated electron systems. Non-resonant inelastic X-ray scattering (NIXS) provides a complementary means to soft X-ray absorption methods in the study of low-energy excitations. The use of higher-energy X-rays (~ 10 keV) enables bulk sensitive measurements. Modern instrumentation and synchrotron facilities permit experiments with access to transitions not only in the dipole-transition regime but also those of higher-order, providing additional insight into the electronic behavior of materials. This will be illustrated using rare-earth materials and excitations corresponding to M, N and O edges, with emphasis on the sensitivity to $4f$ -occupation in cerium-based materials.

6D4

Resonant inelastic hard X-ray scattering in chemical research

P Glatzel¹

¹European Synchrotron Radiation Facility, Grenoble, France

The large penetration depth of a hard X-ray probe is interesting in a large range of applications in chemical research because of its bulk sensitivity and the compatibility with in-situ conditions. Most hard X-ray techniques, however, address the atomic structure while analysis of the electronic configuration is hampered by the large spectral broadening and only few tools for theoretical analysis are available. We will discuss recent developments in hard X-ray resonant inelastic X-ray scattering (RIXS) [1,2] in catalysis research (oxidation of CO over Pt nanoparticles [3]) and coordination chemistry. Multiple scattering (FEFF84) and density functional theory (ORCA, Wien2k) codes have been used to model the experimental data. We find that many spectra can be modeled using a surprisingly simple approach to RIXS. This allows for a detailed analysis of the electronic structure. The limitations of this approach are discussed.

[1] P. Glatzel and U. Bergmann, "High resolution $1s$ core hole X-ray spectroscopy in $3d$ transition metal complexes - electronic and structural information", *Coord. Chem. Rev.* **249** 65-95 (2005)

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[3] P. Glatzel, J. Singh, K.O. Kvashnina and J.A. van Bokhoven, "In situ characterization of the $5d$ density of states of Pt nanoparticles upon adsorption of CO", *J. Am. Chem. Soc.* **132** 2555-2557 (2010)