O 106: Electronic Structure of Surfaces: Spectroscopy, Surface States III

Time: Friday 10:30–13:00 Location: WIL C107

O 106.1 Fri 10:30 WIL C107

ARXPS investigations on surface composition and electronic structure of oxygen- and sulfur-functionalized ionic liquids — •Bettina Heller[1], Claudia Kolbeck[1], Inga Niedermaier[1], Sabine Dommer[2], Nicola Taccardi[3], Jürgen Schatz[2], Peter Wasserscheid[3], Hans-Peter Steinrück[1], and Florian Maier[1] — [1]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Organische Chemie I, FAU Erlangen-Nürnberg, Germany — [3]Lehrstuhl für Chemische Reaktionstechnik, FAU Erlangen-Nürnberg, Germany

Angle-resolved X-ray photoelectron spectroscopy (ARXPS) is a powerful technique to investigate electronic and surface properties of ionic liquids (ILs).[1] This study focuses on sulfur- and oxygen-functionalized ILs, such as thioether and alkoxy ILs, which have the potential of forming carbene complexes used in e.g. catalysis.

With our new Dual Analyzer System for Surface Analysis (DASSA), we simultaneously record ARXPS measurements at 0° (bulk sensitive) and 80° emission (surface sensitive).[2] These spectra provide information on the electronic structure -by means of chemical shifts- and on surface orientation effects.

Imidazolium ILs with ether- and methoxy-sidechains have a random surface orientation in contrast to their non-functionalized ILs counterparts. Regarding the functionalization with sulfur as a thiouronium, a change in the electronic structure of the imidazolium ring is observed.

[1] H.-P. Steinrück, Phys. Chem. Chem. Phys. 2012, 14, 5010.

[2] I. Niedermaier et al., Rev. Sci. Instrum. 2016, 87, 045105.

O 106.2 Fri 10:45 WIL C107

Circular Dichroism in Soft X-ray Photoelectron Diffraction — •Katerina Medjanik[1,2], Gunnar Öhrwall[2], Olena Fedchenko[1], Sergey Chernov[1], Anna Zaporozhchenko-Zymaková[1], Andreas Oelsner[3], Benedikt Schönhense[4], Hans- Joachim Elmers[1], and Gerd Schönhense[1] — [1]Univ. Mainz — [2]MAX IV Lund — [3]Surface Concept GmbH Mainz — [4]Imperial College London

The interference patterns in the angular distribution of electrons from core levels due to *photoelectron diffraction (PED)* give valuable information on the short-range order around the emitter atom. For circularly polarized excitation, the *PED* patterns contain sizeable *circular dichroism in the angular distribution (CDAD)*, originating from the interference of final-state partial waves with different quantum numbers m_l [1]. Since a large region in k-space is observed simultaneously, momentum microscopy is ideal for the study of *CDAD* in *PED*. ToF (time-of-flight) energy discrimination [2] provides simple means for the selection of the desired core level even at very high photon pulse rates (here 100 MHz). We report first results for W(110) and Ir(111) taken at beamline I1011 at MAX II, Lund, Sweden. The diffraction patterns reveal pronounced dichroism in 4f core-level emission. The asymmetry maps A_{CDAD} (k_x,k_y,hv) vary strongly with photon energy between hv=300 and 1000 eV. Funded by BMBF (05K13UM2). [1] Fecher et al., JESRP **122**, 157 (2002); [2] Schönhense et al., JESRP **200**, 94 (2015).

O 106.3 Fri 11:00 WIL C107

Bulk-Sensitive Band Mapping of Mo in the *Tender* X-ray Range — •Dmitry Vasilyev[1], Katerina Medjanik[1], Martin Ellguth[1], Sergey Babenkov[1], Anna Zaporozhchenko-Zymaková[1], Christian Tusche[2], Arndt Quer[3], Florian Diekmann[3], Sebastian Rohlf[3], Matthias Kalläne[3], Kai Rossnagel[3], Yves Acremann[4], Dmytro Kutnyakhov[5], Wilfried Wurth[5], Jens Viefhaus[5], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]Univ. Mainz — [2]FZ Jülich — [3]Univ. Kiel — [4]ETH Zurich — [5]DESY Hamburg

Recent experiments and calculations have demonstrated that ARPES can still be performed in the X-ray range [1]. Intrinsic and extrinsic effects pose limits to the performance of this new approach: the cross section drops rapidly with increasing photon energy, direct transitions are suppressed by inelastic scattering, and the photon momentum causes a sizeable shift of the emission pattern. With increasing kinetic energy the emission angles shrink so that classical ARPES reaches its limits of angular resolution, and the required energy resolution (towards 10^5) is at the technical limit of present instruments. Here, we demonstrate that momentum-microscopy with parallel ToF energy analysis indeed opens the range beyond soft X-rays (i.e., the *tender* X-ray regime) for high-resolution bulk band mapping. Sharp k-patterns with pronounced high contrast have been measured (even for fully oxidized surfaces) up to kinetic energies of 1700 eV at the high-brilliance beamline P04 (PETRA III) for the medium-Z bcc metal Mo. [1] Gray et al., Nat. Mat. **10**, 759 (2011).

O 106.4 Fri 11:15 WIL C107

Oxygen-2*p* valence band dispersion of two-dimensional oxide quasicrystal — •Cheng-Tien Chiang[1,2], Martin Ellguth[2,3], Florian O. Schumann[1], Christian Tusche[2,4], Stefan Förster[1], Richard Kraska[1], Jürgen Kirschner[2,1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [3]Institut für Physik, Johannes-Gutenberg-Universität Mainz, Mainz, Germany — [4]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Jülich, Germany

Valence bands of ultrathin $BaTiO_3$-derived oxide quasicrystal (OQC) on Pt(111) [1] are investigated by angle-resolved photoelectron spectroscopy using the momentum microscope [2]. At around 4 and 6 eV below the Fermi level we observe valence states with flat dispersion as a function of the momentum parallel to the surface, whereas a strongly dispersive feature from 4.6 to 6 eV is discovered along the $[\overline{1}10]$ direction. By comparison with the bulk $BaTiO_3$ band structure we attribute these states to the O-2p valence bands of OQC and discuss their characteristic dispersion.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature **502**, 215 (2013) [2] C. Tusche, A. Krasyuk, and J. Kirschner, Ultramicroscopy **159**, 520 (2015)

O 106.5 Fri 11:30 WIL C107

Non-contact and non-destructive surface analytical tool - The Kelvin Probe: Basics to recent advances — •Subrahmanyam Aryasomayajula — Department of Physics, Indian Institute of Technology Madras, Chennai 600036 India

The surface of metals and semiconductors pose unique challenges in their understanding. Most of the surface analytical tools do modify the surfaces. The Kelvin probe is a most powerful non-contact and non-destructive analytical tool for surface engineering of the metal and semiconductor surfaces; the surface remains virgin even after the measurement. The Kelvin probe technique measures the surface work-function (which is sensitive to the surface preparation). The technique has the unique advantage to follow the real time changes that are taking place on the surface. The Kelvin probe technique is so versatile, it is being employed in several areas: electronic behavior of surfaces of metals and semiconductors,tribology, inter-facial phenomena, adhesion, corrosion,electro-chromic behavior, surface defects and morphology and bacterial bio-film adherence etc,. The present work describes the basics and explores new areas like the failure analyses of corrosion in bio-medical implants (semiconductor - bio-fluid interactions).

O 106.6 Fri 11:45 WIL C107

spectroscopic imaging STM study on Dirac line node material ZrSiS — •qingyu he — max-planck-institute for solid state research, stuttgart, germany

3D Dirac semi-metals have attracted wide interest in recent condensed matter research. The related Dirac line node materials come into focus due to properties such as unconventional magneto-transport and their potential to host topologically nontrivial phases. The non-symmorphic material ZrSiS is one of the first discovered materials of this new family, hosting a nodal line and an unconventional surface state. [1]

Spectroscopic imaging scanning tunneling microscopy (SI-STM) has been a highly valuable technique to study the electronic structure with high energy resolution. In this presentation, we report the investigation of ZrSiS by SI-STM at the atomic scale, in combination with DFT calculations. Firstly, we succeeded in visualizing the signature of the bulk Dirac line node both in real and momentum space, adding key evidences confirming the nodal line and highlighting its exceptional properties. Secondly, an unconventional surface state related to the breaking of non-symmorphic symmetry was observed and its dispersion relation was mapped. Finally, we also discovered the spectroscopic signatures of a type-II Dirac fermion hosted by the surface state.

Our result has impact beyond ZrSiS, providing crucial insights into the Dirac line node materials and non-symmorphic crystals as well.

[1] Schoop, L. M. et al. Dirac cone protected by non-symmorphic symmetry and three-dimensional Dirac line node in ZrSiS. Nat. Commun. 7:11696

O 106.7 Fri 12:00 WIL C107

ERO modelling of surface morphology effect on metals erosion at PSI-2 facility — •Alina Eksaeva[1,2], Evgeny Marenkov[2], Dmitry Borodin[1], Arkadi Kreter[1], Daisuke Nishijima[3], Andreas Kirschner[1], Tobias Schlummer[1], Juri Romazanov[1], Albrecht Pospieszczyk[1], and Stephan Ertmer[1] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung, 52425 Jülich, Germany — [2]National Research Nuclear University MEPhI, 31, Kashirskoe sh., 115409, Moscow, Russia — [3]Center for Energy Research, University of California at San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0417, USA

Linear plasma device PSI-2 with its continuous plasma operation is an excellent test bed for the investigation of plasma-facing material erosion including delicate effects like e.g. nano- and micro-scale surface structures and roughness. However, numerical modelling is indispensable for the correct interpretation of experiments. The 3D Monte-Carlo code ERO is a powerful and versatile tool for describing the erosion and local transport of impurities taking into account the particular geometry. The aim of this work is to incorporate the effect of surface morphology into the ERO modelling first based on free parameters matched with the experiments. Several experiments have already been carried out in PSI-2 facility to investigate the evolving surface morphology of tungsten (W) and chromium (Cr) and provide a consistent set of data for the interpretation with the ERO code. Generally, ERO simulation results are in a good agreement with the experiments.

O 106.8 Fri 12:15 WIL C107

ERO modelling of surface morphology effect on metal erosion at PSI-2 linear plasma facility — •Alina Eksaeva[1,2], Dmitry Borodin[1], Arkadi Kreter[1], Daisuke Nishijima[3], Tobias Schlummer[1], Albrecht Pospieszczyk[1], Stephan Ertmer[1], Andreas Kirschner[1], Juri Romazanov[1], and Evgeny Marenkov[2] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung, 52425 Jülich, Germany — [2]National Research Nuclear University MEPhI, 31, Kashirskoe sh., 115409, Moscow, Russia — [3]Center for Energy Research, University of California at San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0417, USA

Linear plasma device PSI-2 with its continuous plasma operation is an excellent test bed for the investigation of plasma-facing material erosion including delicate effects like e.g. nano- and micro-scale surface structures and roughness. However, numerical modelling is indispensable for the correct interpretation of experiments. The 3D Monte-Carlo code ERO is a powerful and versatile tool for describing the erosion and local transport of impurities taking into account the particular geometry. Several experiments have already been carried out at PSI-2 facility to investigate the evolving surface morphology of tungsten (W) and chromium (Cr) and utilizing various measurement technics provide a consistent set of data for the interpretation with the ERO code. The aim of this work is to incorporate the effect of surface morphology into the ERO modelling based on free parameters matched with the experiments. This approach allows to reproduce the qualitative effects observed and understand their interplay.

O 106.9 Fri 12:30 WIL C107

Untersuchung der Rückhaltemechanismen von Wasserstoff in Beryllium Wolfram Verbindungen — •Michael Eichler, Timo Dittmar und Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

In den experimentellen Fusionsreaktoren JET und zukünftig auch ITER besteht die erste Wand im Hauptraum aus Beryllium (Be). In Bereichen der höchsten Wärmelasten (Divertor) wird zusätzlich Wolfram (W) verwendet. Als Brennstoff werden die Wasserstoffisotope Deuterium (D) und Tritium (T) eingesetzt. Durch den Kontakt der Reaktorwand mit den D- und T-Ionen wird unter anderem das Oberflächenmaterial erodiert und an anderen Stellen deponiert. Dadurch entstehen Be-W Verbindungen. Da das radioaktive T während des Reaktorbetriebs in der Wand eingelagert wird, ist die Untersuchung des Wasserstoffinventars, insbesondere der Rückhaltemechanismen in Be-W Legierungen von besonderem Interesse. Dazu wird das Ultra Hoch Vakuum Experiment namens ARTOSS vorgestellt, welches verschiedene Oberflächenanalytiken vereint und somit die in situ Präparation und Analyse entsprechender Materialien unter wohldefinierten Bedingungen ermöglicht. Der Ionenbeschuss im Reaktor wird mit einer Ionenquelle simuliert. Mit Spannungen bis maximal 20 kV werden D und Wasserstoffionen in Be-W Verbindungen implantiert. Ausserdem werden erste Untersuchungen mittels Röntgenphotoelektronenspektroskopie (XPS), thermischer Desorptionsspektroskopie (TDS) und nuklearer Resonanzanalyse (NRA) gezeigt.

O 106.10 Fri 12:45 WIL C107

First-principles calculations on the surface and bulk electronic structure of TaAs — •Minkyu Shim[1], Jae Hyun Bae[1,2], Jisoon Ihm[1,3], and Cheol-Hwan Park[1] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, South Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, South Korea — [3]Department of Physics, Pohang University of Science and Technology, Pohang 37673, South Korea

Weyl semimetals are a new class of materials whose low-energy electronic excitations are described by the Weyl equation. In this presentation, we discuss the electronic structure of one of the most commonly-known Weyl semimetals, TaAs [1,2], obtained through first-principle calculations. We analyze both the bulk and Fermi arc states of this material. Our work presents a comprehensive understanding of the topological surface states of TaAs, which would be helpful for future experimental studies. The first two authors contributed equally to this work.

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[1] H. Weng, C. Fang, Z. Fang, B. A. Bernevig and X. Dai, Phys. Rev. X 5, 011029 (2015). [2] S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, S. Jia, A. Bansil, H. Lin and M. Z. Hasan, Nat. Commun. 6, 7373 (2015)