O 8: Surface State Spectroscopy I

Time: Monday 10:30–13:00   Location: H4

O 8.1   Mon 10:30   H4

One-step theory of two-photon photoemission — ●Jürgen Braun[1], Roman Rausch[2], Michael Potthoff[2], Jan Minar[1], and Hubert Ebert[1] — [1]LMU München — [2]Universität Hamburg

A general theoretical framework for the description of pump-probe photoemission is presented. The approach is based on a general formulation using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives the system out of equilibrium. The final state is represented by a time-reversed low-energy electron diffraction (LEED) state. The formalism allows for a quantitative calculation of the time-dependent photocurrent that results from core or valence-band excitations, and is applicable to simple metals or more complex materials like topological insulators. Our approach covers as a special case the two-photon photoemission (2PPE) scenario where both the pump-pulse and the probe pulse are weak in intensity. We present as a first application of our fully relativistic implementation within the Munich SPR-KKR package [2] calculated 2PPE spectra from Ag(100), where the first image state serves as intermediate state to probe the occupied bandstructure below the Fermi level [3].

1. J. Braun, R. Rausch, M. Potthoff, J. Minar, H. Ebert, Phys. Rev. B 91, 035119 (2014)
2. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2012)
3. J. Braun, R. Rausch, M. Potthoff, J. Minar, H. Ebert, submitted

O 8.2   Mon 10:45   H4

Tempereture dependent one-step model of ARPES: effects of spinfluctuations and phonons — ●Jan Minar[1,2], Sergey Mankovsky[1], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Various technical developments widened the potential of angle-resolved photo-emission (ARPES) tremendously during the last one or two decades. In particular improved momentum, energy and spin 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. Here, we present a generalization of the state of the art description of the photoemisison process, the so called one-step model that describes excitation, transport to the surface and escape into the vacuum in a coherent way. In particular, we present an theoretical description of the temperature dependent ARPES with the emphasis on spin fluctuations. Effects of finite temperatures are included by the so called alloy analogy model (based on the coherent potential approximation) which allows to describe uncorrelated lattice vibrations in combination with spin fluctuations on the same footing.

Invited Talk   O 8.3   Mon 11:00   H4

Momentum Microscopy with Time-of-Flight Analysis and Spin Filtering: Direct Imaging of k-Space Objects and Spin Textures — ●Gerd Schönhense — Institut für Physik, Johannes Gutenberg-Universität, 55128 Mainz, Germany

Momentum microscopy has recently set impressive benchmarks, in particular in combination with an imaging spin filter [1]. In Mainz we develop a modified approach based on time-of-flight parallel energy detection instead of dispersive analyzers [2]. A fast delay-line detector (> 5 Mcps, 150 ps resolution) provides 3D data recording. The state of development and first scientific results will be reported. The spin-filtered mode was explored at BESSY II (U125-2 NIM) for determination of $P(E_B,k_x,k_y)$ spin textures with more than 10^4 data points simultaneously. Surface and bulk bands of the topological ferroelectric GeTe(111) show Rashba-type spin textures [3]. For W(110) three surface bands with anomalous spin textures were found [4], one of which has been studied before [5]. In the soft-X range (PETRA III, P04) we observed sharp 3D band patterns with giant CDAD asymmetries for Ir and W up to hv=1300eV at T=30K, with 10^5-10^6 data voxels simultaneously. Variation of photon energy yielded $I(E_B,k_x,k_y, k_z)$ datasets for Fermi surface tomography. Strategies to utilize multibunch modes are explored at MAXLAB (Lund, Sweden).

[1] Tusche et al., Ultramicroscopy DOI: 10.1016/j.ultramic.2015.03.020 (2015); [2] Schoenhense et al., JESRP 200 (2015) 94 ; [3] Elmers et al., this conf.; [4] Kutnyakhov et al., this conf.; [5] Miyamoto et al., PRL 108 (2012) 066808.

O 8.4   Mon 11:30   H4

Fast Band-Mapping in the Soft X-Ray Range Using ToF Momentum Microscopy — ●K. Medjanik[1,2], O. Fedchenko[1], S. Chernov[1], D. Kutnyakhov[1], B. Schönhense[3], M. Ellguth[1], A. Oelsner[4], S. Däster[5], Y. Acremann[5], T. Peixoto[6], P. Lutz[6], C.-H. Min[6], F. Reinert[6], J. Viefhaus[7], W. Wurth[8,9], H.J. Elmers[1], and G. Schönhense[1] — [1]Institut für Physik, Uni-Mainz — [2]MAX IV Lab., Lund, Sweden — [3]Imperial College, London, UK — [4]Surface Concept GmbH — [5]ETH Zürich — [6]EP 7, Uni-Wuerzburg — [7]DESY, Hamburg — [8]CFEL, Uni-Hamburg — [9]Desy Photon Science

We present the first results of time-of-flight k-microscopy [1] using soft X-rays. The full 3D Brillouin zones of W and Ir were mapped at beamline P04 of PETRA III between hv=300 and 1300eV. Parallel acquisition of k-discs with 18,000 data points each and about 100 energies resulted in orders of magnitude higher speed and allowed us to operate the monochromator down to its resolution limit of 40,000 at 1000eV. The band features are sharp up to 1300eV at T=30K. Transfer of photon momentum manifests in the form of a rigid shift of the k_x,k_y-patterns and corresponding energy shift. The 40-bunch mode of PETRA provides an ideal pulse period of 192 ns. In order to adapt the ToF-microscope to multibunch conditions or to pump-probe conditions with low-repetitive lasers, a fast electrostatic chopper is developed [2].

Funded by BMBF (05K13UM2, 05K13GU3)

[1] G.Schönhense et al., JESRP 200 (2015) 94-118; [2] A. Zaporozhchenko et al., DPG 2016.

O 8.5   Mon 11:45   H4

The Adsorption Structure of Cobalt Tetraphenylporphyrin on Ag(100) — ●Daniel Wechsler, Quratulain Tariq, Matthias Franke, Liang Zhang, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

Knowledge about the adsorption structure of large organic molecules on single-crystal surfaces is crucial to control how molecules self-assemble on surfaces. We have studied the adsorption structure of cobalt(II) 5,10,15,20-tetraphenylporphyrin (CoTPP) deposited on Ag(100) with low energy electron diffraction (LEED), synchrotron-radiation photoelectron spectroscopy (SRPES), X-ray standing wave (XSW) and near edge X-ray absorption fine structure (NEXAFS). Differences in the LEED patterns show a coverage-dependent unit cell change. From SRPES, XSW and NEXAFS, we were able to determine the atomic height with respect to the surface, the rotational angle of the phenyl rings, and the distortion of the macrocycle. The project is supported by the DFG through FOR 1878 (funCOS).

O 8.6   Mon 12:00   H4

Ab initio core-level spectroscopy for large systems: Comparison of ground-state density-functional based approximations — ●Georg S. Michelitsch, Katharina Diller, Reinhard J. Maurer, and Karsten Reuter — Technische Universität München

Core-level spectroscopy experiments such as Near-Edge X-Ray Absorption Fine-Structure (NEXAFS) allow to sensitively probe the electronic states of gas-phase and surface-adsorbate systems. Particularly for surface-adsorbate systems the complexity of the experimental signatures requires independent first-principles calculations for a reliable analysis. For corresponding system sizes, numerically efficient core-level constraining approaches based on density-functional theory (DFT) are presently the method of choice. Different flavors of this approximate approach vary by different occupations of both the initial core level and the final virtual orbital participating in the electron excitation processes. We systematically benchmark these flavors against experimental K-edge data from a library of organic compounds representing building blocks of organic adsorbates like benzene or porphine. Assessing different DFT functionals, we generally find relative peak positions in the near-edge region to already be well reproduced at the semi-local level. With respect to the different flavors the transition potential approach [1] consistently yields most reliable transition energies and intensities.

[1] L. Triguero, L.G.M. Petterson, and H. Agren, Phys. Rev. B 58,

8097 (1998).

O 8.7   **Mon 12:15**   **H4**
Edge states at vacancy islands on pristine Ni(111) — •Martin Schmitt[1], Jeannette Kemmer[1], Matthias Vogt[1], Matthias Bode[1], Mara Gutzeit[2], Paolo Ferriani[2], and Stefan Heinze[2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität zu Kiel, Leibnizstr. 15, 24098 Kiel, Germany

Recently, the dispersion relations of surface electronic states of pristine Ni(111) has been probed by quasiparticle interference (QPI) [1]. In agreement with earlier inverse photoemission experiments [2] an exchange-split and upward dispersing Shockley-type *sp*-derived surface state was observed. In a follow-up investigation we have studied the electronic properties of step edges surrounding hexagonally shaped vacancy islands by means of low-temperature scanning tunneling spectroscopy. Our results indicate that *A*- or *B*-steps are markedly different. While one type of step edge is essentially featureless, local tunneling spectra measured on the other exhibit an additional peak. By comparison with density functional theory calculations we discuss if this peak can potentially be interpreted as a one-dimensional edge state.

[1] A. Krönlein *et al.*, Phys. Rev. B **89**, 155413 (2014).
[2] M. Donath *et al.*, Phys. Rev. Lett. **70**, 2802 (1993).

O 8.8   **Mon 12:30**   **H4**
Polaron driven structural reconstruction in Rutile $TiO_2(110)$ — •Michele Reticcioli[1], Xianfeng Hao[2], Martin Setvin[3], Ulrike Diebold[3], and Cesare Franchini[1] — [1]University of Vienna — [2]Yanshan University — [3]Vienna University of Technology

The role of polarons in TiO_2 is of key importance for understanding the fundamental properties and functionalities of this material. In this work we use density functional theory with an on-site Coulomb interaction U and molecular dynamics to study the formation and dynamics of small polarons in the reduced rutile $TiO_2(110)$ surface. Our theoretical results are validated by a direct comparison with STM data. We show that excess electrons donated by oxygen vacancies (V_O) form small polarons preferentially in subsurface Ti sites, and that polarons easily hop to neighboring sites in the subsurface and surface layers.

The polaron stability (in terms of the polaron formation energy) has been examined as a function of V_O concentration (5.5%, 11%, 16.6% and 22.2%) by adopting a large (9×2) supercell. It is found that polaron formation become more favorable by increasing V_O concentration due to the lower energy cost to distort the lattice, which is needed to provide the lattice with the necessary flexibility to host self-trapped electrons. At high polaron concentration the polaron-polaron repulsion weakens this trend and drives the system towards an instability, falling into a reconstruction of the surface. The polaron driven surface reconstruction has been studied for two particular suggested structures, named Ti_2O_3-(1×2) and Ti_2O-(1×2). Hence the convenience of the reconstruction with respect to the thermodynamic conditions has been clarified.

O 8.9   **Mon 12:45**   **H4**
Evidence for an extremely low-lying electron-hole excitation mode in the Sb(111)-phonon dispersion measured by HAS — •Patrick Kraus[1], Florian Apolloner[1], Christian Gösweiner[1], Giorgio Benedek[2,3], and Wolfgang E. Ernst[1] — [1]Institute of Experimental Physics, Graz Univerity of Technology, Graz, Austria — [2]Donostia International Physics Center (DIPC), San Sebastian/Donostia, Spain — [3]Dipartimiento di Scienza dei Materiali, Universita di Milano-Bicocca, Milano, Italy

The semimetal antimony (Sb) is an attractive candidate for studying the properties of topological surfaces. Quite recently the surface phonon dispersion curve of Sb(111) as well as the influences of electron-phonon interactions were calculated using DFPT. However, there has been a shortage of experimental data for comparison and verification of the models used. Hence, measurements on antimony are long overdue. As a surface sensitive technique, Helium Atom Scattering (HAS) allows investigating elastic as well as inelastic phenomena associated with structure and dynamics of the electronic corrugation slightly above the Sb(111) surface. Besides confirming the expected surface phonon dispersion curves, recent inelastic HAS measurements on Sb(111) revealed multiple unexpected branches. One of them, lying completely below the Rayleigh curve of the phonon dispersion with a maximum energy at the K-point below 3*meV, can not be assigned to any known feature up to now. The electronic peculiarities in the case of Sb(111) can lead to the formation of defined electon-hole excitation branches which may be detected via iHAS measurements.