O 71: Electronic Structure of Surfaces I

Time: Wednesday 15:00–17:30 Location: REC C 213

Invited Talk O 71.1 Wed 15:00 REC C 213

Detection of strong interaction between electrons and antiferromagnetic magnons in $Ba_{1-x}K_xMn_2As_2$ — Tianlun Yu[1], Rui Peng[1], Guanghan Cao[2], •Haichao Xu[1], and Donglai Feng[1] — [1]Laboratory of Advanced Materials, State Key Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai 200438, People's Republic of China — [2]Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China

The behavior of itinerant carriers under an antiferromagnetic background is critical for many novel physics. K-doped $BaMn_2As_2$ hosts an robust antiferromagnetic order and strong Mn local moments in its highly hole doped metallic state. Here we revealed the band structure by angle-resolved photoemission spectroscopy, and a kink in dispersion is observed at Fermi energy. The coupling constant from self-energy analysis reveales an extremely strong coupling between the itinerant holes and antiferromagnetic magnons. The evolution of the Fermi surface volume with the hole doping follows the Luttinger theory of a normal metal, which rules out a simple half-metal picture of the itinernt ferromagnetism. The large mass enhancement of the As 4p holes by the electron-magnon coupling may be responsible for the emergent itinereant ferromagnetism.

O 71.2 Wed 15:30 REC C 213

Computation of photoelectron matrix elements for angle-resolved photoemission spectroscopy from first principles — •Ji Hoon Ryoo[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Despite the ever-growing role of photoemission spectroscopy in investigating electronic structure of molecules, bulk crystals and their surfaces, calculation of photoemission intensities is, although possible, considered far more difficult than conventional calculations of electronic structures near the Fermi energy. The main reason for the difficulty lies in obtaining electronic structure at energies far higher than the vacuum level, and thus photoelectron states are often approximated as plane-wave-like states [1]. However, several calculations using the KKR method or the embedding method (e.g., Ref. 2 and 3, respectively) have shown that in many cases a more realistic description of photoelectron states beyond the plane-wave approximation is necessary for interpreting the results of spin- and angle-resolved photoemission experiments. We discuss a different method of computing photoemission matrix elements that incorporates final-state effects from first principles.

[1] Z.-H. Zhu et al., Phys. Rev. Lett. 110, 216401 (2013).
[2] J. Sánchez-Barriga et al., Phys. Rev. X 4, 011046 (2014).
[3] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017).

O 71.3 Wed 15:45 REC C 213

The one-step model of time-dependent photoemission combined with time-dependent density functional theory — •Jürgen Braun, Sergiy Mankovsky, and Hubert Ebert — Department Chemie, LMU München

Our fully relativistic one-step model approach to time-resolved photoemission aims at a quantitative description of time-dependent spectroscopic properties of specific solid systems under consideration [1]. The formalism allows for the inclusion of static correlation effects within the LSDA+DMFT approach as well as for the inclusion of a time-dependent potential V(**r**,t), which in principle is available from TDDFT. We used the Elk code [2] to calculate spin- and time-dependent potentials and corresponding occupation numbers for ferromagnetic Fe and Co. These objects, which serve as input quantities for our spectroscopical analysis, represent the feed back of the system generated by a pump pulse. The calculations are compared to corresponding pump-probe experiments.

[1] J. Braun and H. Ebert, Relativistic theory of 2PPE from ferromagnetic materials, Phys. Rev. B **98**, 245142 (2018)

[2] Elk.sourceforge.net: K. Dewhurst, S. Sharma, L. Nordström, O. Granas, E.K.U. Gross et al. (2019)

O 71.4 Wed 16:00 REC C 213

Co on W(110): Spin-dependent interface effects in the electronic structure — •Marcel Holtmann[1], Pascal J. Grenz[1], Eike F. Schwier[2], Shiv Kumar[2], Koji Miyamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

The surface of W(110) exhibits a topologically nontrivial Dirac-cone like state within a spin-orbit induced symmetry gap [1, 2]. When depositing ultrathin Fe films, the state was found to behave differently depending on the film thickness, allowing for manipulation of the "Dirac-fermion mass" via magnetic influence [3]. In order to systematically study the impact of the magnetic adsorbate material, we have investigated the influence of cobalt on the occupied band structure of W(110). In this talk, I will be presenting our results on the preparation of Co/W(110) as well as spin-resolved measurements of the occupied band structure. As in the case of Ni/W(110), we observed growth in the Nishiyama-Wassermann mode. No alteration of the dispersion behavior of the Dirac-cone like surface state was observed - the state gradually fades away with increasing film thickness. Close to the Fermi energy we detected Co-induced interface states, which show Rashba-type spin splitting for submonolayer cobalt coverages.

[1] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012) [2] D. Thonig *et al.*, Phys. Rev. B **94**, 155132 (2016) [3] K. Honma *et al.*, Phys. Rev. Lett. **115**, 266401 (2015)

O 71.5 Wed 16:15 REC C 213

Fermi Surface Tomography of Palladium via Momentum Microscopy — •Xin Liang Tan[1], Kenta Hagiwara[1], Ying-Jiun Chen[1,2], Jakub Schusser[3], Vitaliy Feyer[1], Jan Minar[3], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut, Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic

The Fermi surfaces, which describe all thermodynamical and transport quantities of solids, of transition metals are often failed to be modeled by one-electron mean-field theory due to strong correlations among the valence electrons. In addition, relativistic spin-orbit coupling pronounced in heavier elements lifts the degeneracy of the energy bands and further modifies the Fermi surface. Palladium, a 4d metal attributed to both significant spin-orbit coupling and electron correlations, is ideal for a systematic and fundamental study on the two fundamental physical phenomena and their interplay in electronic structure. In this talk, we will explore the experimentally determined electronic structure of palladium in four dimensional energy-momentum space ($E_{Binding}$,k_x,k_y,k_z) obtained via constant initial-state momentum microscopy. The complete 3D-Fermi surface of palladium and corresponding isoenergy surfaces at higher binding energies were tomographically mapped with an energy- and polarization-variable light source. Spin-orbit coupling and electron correlations in palladium will be presented in the context of energy-momentum relations across the Fermi surface and isoenergy surfaces.

O 71.6 Wed 16:30 REC C 213

Orbital imaging: Sparsity-driven phase retrieval of angular-resolved photoemission spectroscopy data — •Matthijs Jansen[1], Marius Keunecke[1], Marten Düvel[1], Christina Möller[1], David Schmitt[1], Wiebke Bennecke[1], Jasmin Kappert[1], Daniel Steil[1], Russell Luke[2], Sabine Steil[1], and Stefan Mathias[1] — [1]1st Physical Institute, University of Göttingen, Göttingen — [2]Institute for Numerical and Applied Mathematics, University of Göttingen, Göttingen

In recent years, iterative phase retrieval of angle-resolved photoemission spectroscopy (ARPES) has attracted interest as a method to visualize molecular orbitals in molecule-metal interfaces. This method, dubbed *orbital imaging*, relies on prior knowledge of the investigated orbital. So far, successful orbital imaging has been based on the support constraint, for which the shape of the orbital must be known.

We will present a sparsity-driven approach to phase retrieval, which uses only the number of non-zero pixels in the orbital. This sparsity constraint is easy to determine and independent of the orbital shape. Additionally, we include symmetry in the phase retrieval approach. We apply the resulting phase retrieval algorithms successfully to both

simulated and experimental ARPES data, acquired using a so-called *momentum microscope*, which uses time-of-flight-based detection to measure the full momentum and energy-dependent spectrum in a single measurement. This enables us to image multiple molecular orbitals simultaneously. We conclude that sparsity-driven phase retrieval requires less prior knowledge to achieve good orbital imaging results.

O 71.7 Wed 16:45 REC C 213

Hard X-ray Valence-Band Mapping and Photoelectron Diffraction on InGaMnAs Thin Films — •K. Medjanik[1], A. Winkelmann[2], O. Yastrubchak[3], J. Sadowski[4,5], L. Gluba[6,7], D. Vasilyev[1], S. Babenkov[1], S. Chernov[1], O. Fedchenko[1], H.J. Elmers[1], and G. Schönhense[1] — [1]JGU, Inst. für Physik, Mainz — [2]AGH Univ. of Science and Technology, Krakow, Poland — [3]Inst. of Semiconductor Physics, Kyiv, Ukraine — [4]Inst. of Physics, Warszawa, Poland — [5]Linnaeus Univ., Kalmar, Sweden — [6]Inst. of Agrophysics, Lublin, Poland — [7]Inst. of Physics, Lublin, Poland

The interplay of electronic and geometric structure is one of the key issues of materials research. We present results for the prototypical ferromagnetic semiconductor InGaMnAs (3% In, 2.5% and 5% Mn), recorded at photon energies between 3 and 5 keV at the new beamline P22 at PETRA III (Hamburg) by Time-of-Flight Momentum Microscopy [1]. In the non-centrosymmetric GaAs crystal structure, element-specific hXPD clearly reveals site-specific Ga and As diffraction patterns which are rotated by 90° at identical kinetic energies. The Mn-atoms show diffractograms, which are characteristic for the Ga-sites, as expected for substitutional Mn in GaAs [2]. Sharp valence-band k-patterns show that with increasing Mn-doping the splitting of the p1/2-derived band from the heavy- and light-hole p3/2-bands increases. In addition, the Fermi energy decreases i.e. with increased Mn content the frontier bands are less filled.

[1] K. Medjanik et al., J. of Synchr. Radiation 26, 1996 (2019). [2] T. Dietl & H. Ohno, Rev. Mod. Phys. 86, 187 (2014).

O 71.8 Wed 17:00 REC C 213

Surface electronic structure of Te on Ag(111) and Cu(111) — •Begmuhammet Geldiyev, Jonas Hauner, Janek Rieger, M. Alexander Schneider, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The unoccupied and occupied surface electronic structure of Te on Ag(111) and Cu(111) was studied by bichromatic two-photon photoemission (2PPE) and laser-based one-photon photoemission (1PPE). For 1/3 monolayer of Te a $(\sqrt{3} \times \sqrt{3})R30°$ superstructure forms on Ag(111) in contrast to the $(2\sqrt{3} \times \sqrt{3})R30°$ structure on Cu(111) with a doubled unit cell. For both surfaces two occupied bands are found by 1PPE and one unoccupied surface band by 2PPE. For Te/Cu(111) the higher-lying occupied band is split into two bands for the inequivalent directions of the doubled unit cell. All bands on Cu(111) are shifted up in energy compared to Ag(111) in agreement with density-functional-theory calculations. The orbital character of the electronic bands is probed by polarization-dependent measurements in normal emission. On Te/Ag(111) time-resolved 2PPE measurements yield a lifetime of $\approx$ 31 fs for the unoccupied state located $\approx$ 0.53 eV above the Fermi level, which has an electron-like dispersion. For the analogous surface state on Cu(111) at $\approx$ 1.43 eV no measureable lifetime was found.

O 71.9 Wed 17:15 REC C 213

Double photoemission spectroscopy of $SrTiO_3$(001) using a high-order harmonics light source — •Robin Kamrla[1], Cheng-Tien Chiang[1], Andreas Trützschler[1], Michael Huth[2], Frank Oliver Schumann[2], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Photoelectron spectroscopy (PES) has provided deep insights into the electronic structure of solids. However, correlation effects can only be addressed indirectly. To observe such phenomena directly, double photoemission (DPE) spectroscopy is able to detect pairs of correlated photoelectrons that are emitted upon absorption of a single photon [1]. In this contribution we present PES and DPE data for $SrTiO_3$(001), obtained by a laboratory high-order harmonic (HHG) light source at $h\nu = 25.2$ and 32.4 eV operating at MHz repetition rates. Well-ordered $SrTiO_3$(001) surfaces have been prepared by annealing at 770 K in an oxygen atmosphere of $5 \cdot 10^{-6}$ mbar. PES confirms a TiO_2 terminated surface and reveals a binding energy of the O_{2p} state of 3.2 eV. In DPE we find an onset for emission of correlated photoelectrons at a pair binding energy of 7.5 eV, independent of the individual electron energies. The DPE data will be compared to data for NiO and CoO surfaces, as well as for Ag(001) [2], indicating the presence of a strong electron-electron interaction in $SrTiO_3$.

[1] J. Berakdar et al., Phys. Rev. Lett. **81** (1998)
[2] A. Trützschler et al., Phys. Rev. Lett. **118** (2017)