O 43: Poster Tuesday: Electronic Structure

Time: Tuesday 18:00–20:00 Location: Poster D

O 43.1 Tue 18:00 Poster D

Studying the type-II Weyl semimetal candidate *Td*-WTe_2 with two-photon photoemission — •Petra Hein[1], Stephan Jauernik[1], Yulin Chen[2], Lexian Yang[2], Binghai Yan[3], Claudia Felser[3], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Germany — [2]Physics Department, Tsinghua University, Beijing, China — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Laser-based angle-resolved photoemission spectroscopy (ARPES) and two-photon photoemission (2PPE) are combined to investigate the near-E_F electronic structure of the type-II Weyl semimetal candidate WTe_2.

Using a widely tunable femtosecond laser system, we are able to access a variety of both occupied and unoccupied electronic states. Initial, intermediate and final states can be clearly distinguished via their characteristic peak shift in dependence of the photon energy. Photon-energy scans in conventional ARPES studies of three-dimensional systems are typically used to determine the k_z dispersion of the occupied band structure. Here we show that in an analogous manner 2PPE is capable of probing the k_z dispersion of unoccupied bands between E_F and the vacuum level. The results are compared to different band structure calculations and current ARPES studies of WTe_2.

O 43.2 Tue 18:00 Poster D

Drumhead Surface States in ZrSiTe — •Andreas Topp[1], Lukas Müchler[2], Raquel Queiroz[3,1], Bettina V. Lotsch[1], Leslie M. Schoop[4], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, DEU-70569 — [2]Flatiron Institute, New York, USA-10010 — [3]Weizmann Insitute of Science, Rehovot, ISR-7610001 — [4]Department of Chemistry, Princeton University, Princeton, USA-08544

ZrSiS, ZrSiTe and related compounds have become of increased interest in recent years. As members of space group 129, their crystal structure contains nonsymmorphic symmetry elements in combination with a square-net lattice of atoms. While the nonsymmorphic symmetry is responsible for band crossings at high-symmetry points that are not affected by spin-orbit coupling, the square net produces a Dirac line node forming a diamond-like structure in the first Brillouin zone. ARPES measurements showed additional surface states in ZrSiS that could be explained in the framework of reduced surface symmetry [1]. Here, we focus on the isostructural compound ZrSiTe, which shows an even more complicated surface band structure and explain the emergent surface bands in the context of topological drumhead surface states [2].

[1] Topp et al., Phys. Rev. X 7, 041073 (2017).
[2] Y.-H. Chan et al., Phys. Rev. B 93, 205132 (2016).

O 43.3 Tue 18:00 Poster D

STM-Investigations of Re(0001) suface states — •Johannes Regel[1], Torge Mashoff[1], Jürgen Braun[2], Hubert Ebert[2], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Department Chemie, Ludwig Maximilians-Universität, München

Due to the broken symmetry, the electronic structure of surfaces can differ significantly from the bulk structure. In case of strong spin-orbit coupling, as given in rhenium, this can lead to Rashba spin splitting of the electronic states. Although the strong spin momentum should forbid backscattering, the rhenium surface shows standing waves in the local density of states originating from defects and step edges. We investigate the electronic states of the Re(0001) surface using low temperature scanning tunneling microscopy and spectroscopy. Differential conductivity measurements lead to an energy-dependent analysis of the wavelength, phase and damping of these states. Additionally, we use molecular beam epitaxy to deposit sub-monolayer gold and nickel islands onto the Re-surface and study their influence on the measurements as well as the pseudomorphic growth of these metals. Our results are compared with one-step model calculations of the electronic structure of rhenium and show good agreement.

O 43.4 Tue 18:00 Poster D

On superconducting properties of clean Nb(110) surface and its magnetic adatom-induced Yu-Shiba-Rusinov states — •Artem B. Odobesko, Stefan Wilfert, Robin Boshuis, and Matthias Bode — Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany

We have studied cleaning procedures of Nb(110) by low-energy electron diffraction, Auger electron spectroscopy, and scanning tunneling microscopy and spectroscopy. Our results show that the formation of a surface-near impurity depletion zone is inhibited by the very high diffusivity of oxygen in the Nb host crystal. Oxygen can be removed from the surface by heating the crystal to T $\sim$ 2400°C. Tunneling spectra measured on the clean Nb(110) surface exhibit a sharp conductance peak in the occupied states at an energy of about -450 meV. The clean Nb(110) surface is superconducting with a gap width and a critical magnetic field strength in good agreement to the bulk value. Spatially resolved spectra take in an external magnetic field show a zero-bias anomaly in the vortex core. We will discuss the potential of the Nb(110) surface to serve as a platform for Yu-Shiba-Rusinov bound states inside the superconducting gap when magnetic impurities induce a pair-breaking scattering potential for Cooper pairs [1]. The adsorption site–dependence of the Yu-Shiba-Rusinov states will be explored by atomic manipulation.

[1] B.W. Heinrich, J.I. Pascual, K.J. Franke, Prog. Surf. Sci. textbf93, 1 (2018).

O 43.5 Tue 18:00 Poster D

Spectroscopic signatures of single molecules and their aggregates in the presence of a dielectric surface — •Meral Ari, Oliver Stauffert, and Michael Walter — Institute of Physics, University of Freiburg, Freiburg, Germany

Polycyclic aromatic hydrocarbons promise to be attractive candidates for materials to build the next generation of optoelectronic devices. In order to be able to utilize them at maximum yield, understanding their electronic structure and optical properties is essential. Hereby we are especially interested in acenes. We describe their electronic structures with density functional theory (DFT) and excited state properties with time-dependent density functional theory (TDDFT). Experimentally observed spectroscopic shifts are determined from the effect of the permittivity of the neon surface in a joined effort with the macroscopic QED group of S. Buhmann. The dielectric constant of the neon surface is calculated by using different ab-initio methods and their effects are compared.

O 43.6 Tue 18:00 Poster D

A one-dimensional hole gas in monolayer MoS_2 — •Clifford Murray[1], Wouter Jolie[1,2], Joshua Hall[1], Arkady Krasheninnikov[3,4], Carsten Busse[1,2,5], Hannu-Pekka Komsa[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Department of Applied Physics, Aalto University School of Science, Aalto, Finland — [4]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [5]Department Physik, Universität Siegen, Germany

We epitaxially grow high-quality monolayer molybdenum disulfide (ML-MoS_2) on graphene on Ir(111), which is close to freestanding on this substrate [1]. We probe its electronic structure with low temperature scanning tunnelling spectroscopy.

The valence band is found to undergo stepwise bending at line defects such as 4|4E-type mirror twin boundaries (MTBs) and flake edges. Localised charge in these defects causes an upwards bending of the bands in the surrounding ML-MoS_2 semiconductor. This is experienced particularly strongly in the valence band, and leads to a 1D confinement of the charge carriers (holes) perpendicular to the defect. By contrast, the effect is not seen at 4|4P MTBs, the MTB type commonly present in the analogous $MoSe_2$ monolayer. We seek to understand and describe the observed behavior with the help of density functional theory.

[1] Hall, J. et al., 2D Mater. 5, 025005 (2018)

O 43.7 Tue 18:00 Poster D

Spin effects in the unoccupied electronic structure of Ir(111) and graphene/Ir(111) — •Fabian Schöttke, Katharina T. Ritter, Anke Beck-Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

The electronic structure of iridium surfaces is of interest with respect to spin-orbit interaction at surfaces of heavy elements. Especially the Ir(111) surface is the subject of numerous investigations because it is well suited as a substrate for graphene [1]. A two-photon-photoemission study on graphene/Ir(111) using circularly polarized light reports a Rashba-type spin splitting of the image-potential state [2]. However, this result is put into question by another study [3].

We present an inverse-photoemission study with spin resolution on the unoccupied electronic states of Ir(111) and graphene/Ir(111). We address the spin dependence of the image-potential states for the bare Ir(111) surface and the graphene-covered surface in order to examine the interaction of the substrate with the graphene overlayer.

[1] Varykhalov *et al.*, Phys. Rev. Lett. **108**, 066804 (2012).
[2] Tognolini *et al.*, Phys. Rev. Lett. **115**, 046801 (2015).
[3] Arafune *et al.*, Prog. Surf. Sci. doi:10.1016/j.progsurf.2018.08.001.

O 43.8 Tue 18:00 Poster D

Investigation of honeycomb Na_2IrO_3 surface structures by functionalized STM and STS probes — •Thomas Dziuba[1], Ina Pietsch[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Universität Augsburg, Germany

Na_2IrO_3 is a prototypical Kitaev material in the iridate family, consisting of alternating stacks of negatively charged honeycomb Ir_2NaO_6 layers and positively charged hexagonal Na_3 layers [1]. In addition to its frustrated magnetic bulk properties, Na_2IrO_3 has also been discussed as host of topological electronic surface states. However, since most studies focus on bulk magnetic properties, information on the surface electronic structure is still rather limited. We report a thorough study of the structural and electronic properties of in-situ cleaved surfaces by atomic resolution scanning tunneling microscopy and spectroscopy. Based on our previous study of surface reconstructions [2], we now concentrate our attention on a detailed investigation of the differences between the bulk and surface electronic properties. We deeply study the influence of alkali metal functionalized tips and report the interrelation between surface reconstructions, the local electronic structure and the tip status.

Work supported by DFG through SPP 1666 (Topological Insulators).

References:

[1] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010)
[2] F. Lüpke et al., Phys. Rev. B 91, 041405(R) (2015)

O 43.9 Tue 18:00 Poster D

Evidence for Conducting Na_2IrO_3 Surfaces prepared in UHV — •Sarah Maamar[1], Thomas Dziuba[1], Ina Pietsch[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Universität Augsburg, Germany

Honeycomb iridate Na_2IrO_3 attracts considerable interest as prototype material for the study of the Kitaev interaction [1]. However, first-principles-derived tight-binding model calculations have also proposed topologically nontrivial electronic behaviour in this system, namely 2D Quantum Spin Hall [2] or 3D correlated topological insulator [3] states. Experimental evidence for this is still missing, possibly because of the high reactivity of Na_2IrO_3, leading to rapid degradation of its surface. To overcome this problem, we cleave single crystals in ultra-high vacuum (UHV), evaporate gold contacts and study the electrical conductivity as function of temperature between 100 K and 260 K without breaking the UHV conditions. Linear I-V curves prove ohmic contacts. In contrast to previous resistivity measurements, which displayed insulating behaviour [4], our data indicate a saturation of the resistance at low temperature, i.e. a finite conductivity at 100 K. This work is supported by the DFG through the SPP 1666 (Topological Insulators).

[1] S.M. Winter et al., J. Phys.: Condens. Matter 29, 493002 (2017).
[2] A. Shitade et al., Phys. Rev. Lett. 102, 256403 (2009).
[3] C.H. Kim et al., Phys. Rev. Lett. 108, 106401 (2012).
[4] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010).

O 43.10 Tue 18:00 Poster D

Tunable Surface Band Inversion in Black Phosphorous — •Klara Volckaert[1], Deepnarayan Biswas[1], Brian Kiraly[2], Søren Ulstrup[1], Charlotte Sanders[3], Marco Bianchi[1], Alexander Khajetoorians[2], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]Radboud University, Nijmegen, The Netherlands — [3]Central Laser Facility, Harwell, United Kingdom

Black phosphorous is a semiconductor that is gaining interest due to its tunable bandgap, which is thought to lead to an anisotropic Dirac semimetal upon critical doping with alkalis. Therefore this material could prove relevant to electronic and optoelectronic devices. Here we study the effect of potassium doping on bulk black phosphorous that leads to an elliptical electron-like pocket appearing. The nature of these bands is deduced using the k_z dispersion acquired by means of angle-resolved photoemission spectroscopy (ARPES). Curiously, at high levels of potassium deposition, electron-like states emerge below the Fermi level that have not previously been reported.

O 43.11 Tue 18:00 Poster D

Electronic properties of potassium-doped black phosphorus on the atomic scale — Brian Kiraly, •Elze Jantien Knol, Daniel Wegner, and Alexander Ako Khajetoorians — Scanning Probe Microscopy, Radboud University, Nijmegen, the Netherlands

In 2015 it was proposed that by applying a surface electric field gradient to few-layer black phosphorus, the material can be tuned from a moderate-gap semiconductor into a band-inverted semimetal [1]. Experimentally, it was shown that such a transition can be achieved by adding potassium atoms to the surface [2]. Since then there has been interest in the electronic properties of the surface of black phosphorus and the role of potassium. Here, utilizing low-temperature scanning tunneling microscopy and spectroscopy, we probe the variations in the electronic properties of black phosphorus, with varying surface coverage of potassium at the atomic scale. We discuss the changes to both the band-gap and Fermi energy, in the presence of surface doping. Moreover, we present the effect of charge-mediated interactions on the atomic distribution of potassium atoms, and relate this to the electrostatic screening of black phosphorus.

[1] Q. Liu, X. Zhang, L. B. Abdalla, A. Fazzio, A. Zunger. Nano Lett. 15 (2), 2015.

[2] J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B. G. Park, J. Denlinger, Y. Yi, H. J. Choi, K. S. Kim. Science 349 (6249), 2015.