O 86: Electronic Structure of Surfaces: Spectroscopy, Surface States II

Time: Thursday 15:00–17:30 Location: H2

O 86.1 Thu 15:00 H2

Low temperature STM/AFM detection of 2D electronic gas on reduced $SrTiO_3$ surface — •Akash Gupta, Marcin Kisiel, Remy Pawlak, and Ernst meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Perovskite such as $SrTiO_3$ ubiquitous to host various reconstruction with fine tuning of the annealing temperature. At 1050°C, in oxygen poor conditions, a $\sqrt{5}\times\sqrt{5}$ surface reconstruction is formed with oxygen vacancies. These oxygen vacancies result in compactly confined electrons as two-dimensional electron gas (2DEG) system. The 2DEG is confirmed as filled surface states in Low Temperature (4 K, UHV) Scanning Tunneling Spectroscopy (STS). Additionally, Image Potential States (IPS) emerges at lower energies than vacuum level, revealing work function, as well. The charging of this 2DEG system can be induced with capacitively coupled tip of Atomic Force Microscope, and it results in giant dissipation peaks as signature of surface charging with change in the tip-sample voltage. Furthermore, quantum capacitance is calculated as function of the gate voltage. The evolution of dissipation peaks were observed with tip-sample distance. The Force-Distance curves confirm the 2DEG charging and is used to determine the tunneling rate of the charging within 2DEG system.

O 86.2 Thu 15:15 H2

Tunneling Spectroscopy of RuO_2(110): Electronic Structure, Correlation Effects and Substrate Interactions — •Philipp Kessler, Andreas Feuerpfeil, Hendrik Hohmann, Matteo Dürrnagel, Armando Consiglio, Jonas Erhardt, Michael Sing, Ralph Claessen, Ronny Thomale, and Simon Moser — Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

The (110) surface of RuO_2 hosts a flat band surface state (FBSS) close to the Fermi level that is prone to Fermi surface instabilities and can be readily observed in angle resolved photoemission. A local spectroscopic investigation of this FBSS to study such instabilities is, however, still outstanding. In this talk, we present the synthesis of high quality RuO_2(110) surfaces, enabling systematic scanning tunneling spectroscopy (STS) measurements across wide defect free domains. We observe hints of correlation effects, manifesting in signatures of a charge density wave and a zero-bias anomaly. Furthermore, we offer preliminary evidence suggesting that the electronic structure of RuO_2 depends on the oxide film thickness and immediate screening environment within the substrate. These findings illuminate the interplay between the Ru metal substrate and the RuO_2 oxide, advancing this topical material.

O 86.3 Thu 15:30 H2

Quasi-particle interference studies on ultra-thin films of Cu(111) — •Jungin Yeo — Chung-Ang University, Seoul 06974, Republic of Korea

Recently, ultra-thin crystalline Cu(111) film has been successfully grown on a sapphire substrate through the atomic sputtering epitaxy (ASE). In-depth studies were conducted to explore the crystal growth mechanism and the oxidation process. Ultra-thin film without grain boundary (GB) shows hidden intrinsic nature such as transport by hole carriers. Meanwhile, twin boundaries (TB) appear inevitably during the growth even such an atomically high-quality film. As two orientations adjacent to a TB satisfy the symmetry operation exactly, TBs are expected to show different electronic properties from GBs. The unique electronic properties resulting from the two-dimensional nature and the presence of TBs are currently under investigation. For our study, we utilized scanning tunneling microscopy (STM) to examine 20 nm thick ASE-grown Cu(111) films. The STM topography revealed an atomically flat surface with an indication of twin boundaries. We performed quasi-particle interference (QPI) measurements across TBs. The surface states of Cu(111) and quantum-confined states within the film thickness were successfully resolved. By analyzing the QPI data, we were able to reconstruct the electronic dispersion near the Fermi energy, both at the surface and within the bulk of 20 nm thick. The transmission probability across TBs will be discussed.

O 86.4 Thu 15:45 H2

Electronic structure of the correlated topological metals $CoTe_2$ and $NiTe_2$ — Abhijeet Shelke[1], Chien-Wen Chuang[2], Truc Ly Nguyen[1], Yo-Xun Chen[1], Masato Yoshimura[1], Nozomu Hiraoka[1], Satoru Hamamoto[3], Masaki Oura[3], Chia-Nung Kuo[4], Chin-Shan Lue[4], Atsushi Fujimori[5,1], and •Ashish Chainani[1] — [1]National Synchrotron Radiation Research Center, Hsinchu 300092, Taiwan — [2]Dept. of Physics, Tohoku University, Sendai 980-8578, Japan — [3]RIKEN SPring-8 Center, Hyogo 679-5148, Japan — [4]Dept. of Physics, NCKU, Tainan 70101, Taiwan — [5]Dept. of Physics, The University of Tokyo, Tokyo 113-0033, Japan

The transition-metal(TM) tellurides $CoTe_2$ and $NiTe_2$ are known to exhibit topological semi-metallic Dirac bands from ARPES studies. We carry out core level and valence band measurements using hard x-ray photoemission spectroscopy(HAXPES), x-ray absorption spectroscopy(XAS) and TM $2p-3d$ resonant photoemission spectroscopy(R-PES) to study electronic structure of $CoTe_2$ and $NiTe_2$. The R-PES spectra show clear evidence of TM LVV Auger two-hole correlation satellites. Using the Cini-Sawatzky method, we estimate an on-site Coulomb energy, U_{dd}∼3 eV for Co in $CoTe_2$, and U_{dd}∼4 eV for Ni in $NiTe_2$. Using these values in charge-transfer cluster model calculations, we simulate the TM $2p$ HAXPES core level and L-edge XAS spectra of $CoTe_2$ and $NiTe_2$. The electronic parameter analyses indicate a negative charge transfer energy Δ for both $CoTe_2$ and $NiTe_2$. The results indicate a p-type metal in terms of the Zaanen-Sawatzky-Allen phase diagram for $CoTe_2$ and $NiTe_2$.

O 86.5 Thu 16:00 H2

Visualizing topological ladder in $PtTe_2$ — •Mohammed Qahosh[1], Gustav Bihlmayer[2], Jakub Schusser[3], Muthu Masilamani[3], Friedrich Reinert[3], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]PGI-1/IAS-1 Forschungszentrum-Jülich — [3]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg

We have examined the topological ladder [1] and band inversions in $PtTe_2$ using spin-polarized angle-resolved photoemission (spin-ARPES) with two-dimensional momentum imaging. Examining such spin images allows in-depth insight into the topological properties, not accessible by routine methods. We mapped extended momentum-space regions and visualized distinct topological ladder states, notably a surface Dirac cone at $E_B \sim 2.3$ eV, as well as states at $E_B \sim 1.0$ eV, $E_B \sim 1.6$ eV, and near the Fermi level. By comparison to *ab initio* calculations, we demonstrate a significant correlation between the measured and the initial state spin polarization. We discuss interatomic phase shifts [2] for orbitals mixed between Pt and Te sites as well as spin-orbit scattering that leads to additional spin polarization in spin-ARPES. [1] Nature Materials 17, 21 (2018). [2] Phys. Rev. Lett. 130, 146401 (2023).

O 86.6 Thu 16:15 H2

Origin of the Spin-Polarized Fermi Surface of a Tl Bilayer on Ag(111) — •Sven Schemmelmann[1], Yuichiro Toichi[2], Peter Krüger[3], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Applied Physics, Osaka University, Japan — [3]Institut für Festkörpertheorie, Universität Münster, Germany

ARPES measurements have shown that the Fermi surface of a Tl bilayer grown on Ag(111) exhibits two hexagonal-shaped states [1]. While the inner one is fully spin polarized, the outer one appears to be unpolarized. Spin-resolved inverse photoemission experiments of the unoccupied states reveal the origin of this peculiar behavior. We observe two downward dispersing states which are both spin split. The two spin branches of the one state are responsible for the two states observed forming the Fermi surface. Interestingly, the spin up branch coincides with the spin down branch of the other downward dispersing state. This is the reason why this state appears to be unpolarized.

[1] T. Kobayashi *et al.*, Nano Lett. **23**, 7675 (2023)

O 86.7 Thu 16:30 H2

Analyzing excitonic contributions to reflection anisotropy spectra — •Max Grossmann[1], Kai Daniel Hanke[2], Chris Yannic Bohlemann[2], Thomas Hannappel[2], Wolf Gero Schmidt[3], and Erich Runge[1] — [1]Theoretical Physics I, Institute of Physics,

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Reflection anisotropy spectroscopy (RAS) is a powerful optical tool for probing semiconductor surfaces. However, the interpretation of RA spectra is challenging due to the complex interplay of features caused by surface states and so-called surface-induced bulk anisotropy, as well as the significant influence of excitonic effects. Overcoming these challenges requires a close collaboration between experiment and theory. In this work, we combine high-quality low-temperature RAS measurements with state-of-the-art *ab initio* calculations in the framework of many-body perturbation theory to study the RAS of arsenic-terminated Si(100) surfaces. The excitonic contributions to the RAS are studied in detail through a thorough analysis of the results from a solution of the Bethe-Salpeter equation. Our approach aims to combine experimental observations with theoretical insights to decipher the complex effects that shape RAS spectra and to advance the understanding of the optical properties of semiconductor surfaces.

O 86.8 Thu 16:45 H2

Composition and band gap of aluminum alloyed beta-gallium oxide determined by XPS — •Lukas Schewe[1], Jana Rehm[2], Ming-Chao Kao[3], Vedran Vonk[3], Zbigniew Galazka[2], Saud Bin Anooz[2], Andreas Popp[2], and Jan Ingo Flege[1] — [1]Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — [2]Leibnitz-Institut für Kristallzüchtung, Berlin — [3]CXNS-Center for X-ray and Nano Science, DESY Hamburg

Beta-phase gallium oxide is a wide-gap semiconductor with a band gap of 4.85eV and promising prospects in high-power electronics. The electric breakdown field can be increased by alloying the oxide with aluminum, further enhancing its properties.
The present work discusses structural and electronic properties of β-$(Al_xGa_{1-x})_2O_3$ thin films and bulk crystals with Al content of up to 33 %. Their Al content was determined by X-ray photo-electron spectroscopy (XPS) and compared to the values estimated from X-ray diffraction (XRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Additionally, the thin films have been investigated by XPS depth profiling, i.e., XPS combined by sequential Ar^+ sputtering, revealing lower aluminum content at the sample surface, which points to possible surface segregation of gallium during annealing. Furthermore, the band gap was determined by electron loss spectra from XPS and optical absorbance measurements and correlated to the Al content estimated for both thin films and bulk crystals.

O 86.9 Thu 17:00 H2

Higher-order van Hove singularities in Kagome metal RbV_3Sb_5 — •Gahee Lee — Department of Physics, Chung-Ang University, Seoul 06974, Republic of Korea

The divergence of the density of states (DOS) near the Fermi energy is crucial for enhancing electron correlations. Van Hove singularities (vHS) commonly cause this DOS divergence, with their properties determined by the dimensionality of electron dispersion. The atomic arrangement on the surface of layered materials can influence the effective dimensionality of electron dispersion, thereby shaping the characteristics of vHS. In V-based Kagome metals RbV_3Sb_5 (A = K, Rb, and Cs), the saddle-shaped dispersion results in two-dimensional vHS. Interestingly, the surface arrangement of atoms in a Kagome lattice can modify the effective dimensionality of electron dispersion, affecting the strength of electron correlations. In this study, we present a novel approach to enhancing electron correlation by arranging the surface Rb atoms. The resulting higher-order vHS significantly enhances the divergence of DOS and strengthens charge density waves in V-based Kagome metals.

O 86.10 Thu 17:15 H2

Single Hemisphere & Time-of-Flight Hybrid Photoelectron Momentum Microscopy — •Olena Tkach[1], Matthias Schmitt[2,3], Deepnarayan Biswas[2], Olena Fedchenko[1], Jieyi Liu[2], Hans-Joachim Elmers[1], Michael Sing[3], Ralph Claessen[3], Tien-Lin Lee[2], and Gerd Schönhense[1] — [1]JGU Mainz, Germany — [2]DIAMOND, Didcot, United Kingdom — [3]Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

The 2ns pulse period of the photon beams from most synchrotrons is too short for pure time-of-flight (ToF) photoelectron spectroscopy. With the use of a hemispherical analyzer (HSA) as a pre-filter, ToF momentum microscopy becomes possible at such high pulse rates. The first hemisphere & ToF hybrid MM is operated at the soft X-ray branch (photon energies from 105 eV to 2 keV) of beamline I09 at DIAMOND. The HSA reduces the transmitted energy band to typically 0.5 eV, which is then dispersed by ToF recording. In the first experiments the total efficiency gain when switching from the standard 2D (k_x, k_y) to the 3D $(k_x, k_y, E_{\mathrm{kin}})$ hybrid mode was about 25. It is determined by the number of resolved kinetic energies (here 12) and the transmission factor of the electron optics due to the higher pass energy (500 eV) of the HSA in hybrid mode. The α^2- term and the transit time spread due to different path lengths in the HSA are numerically corrected. The performance was validated by studying the well-known electronic structure of Au(111) and Cu(111), including circular dichroism (CDAD) measurements. The high efficiency was exploited in a series of measurements on the Kagome metal CsV_3Sb_5.