

## O 90: Electronic structure of surfaces: Spectroscopy, surface states IV

Time: Thursday 10:30–13:00

Location: MA 042

O 90.1 Thu 10:30 MA 042

**Mahan cone backfolding in Phthalocyanine overlayers on Au(111)** — ●BENITO ARNOLDI, DOMINIK JUNGKERN, JOHANNES SEIDEL, JOHANNES STÖCKL, BENJAMIN STADTMÜLLER, and MARTIN AESCHLIMANN — Department of Physics, TU Kaiserslautern, Erwin-Schrodinger-Strasse 46, 67663 Kaiserslautern, Germany

Here, we extend our previous study of the spin-polarization of Mahan cone transitions of bare noble metals to metal-organic interfaces. For the latter material system, the long range order of the molecular film leads to clear back-folding of the central Mahan cone, i.e., to a scattering of substrate electrons at the molecular films. We employ spin and angle resolved laser ARPES with linear polarized light and 6eV photons to gain insight into the spin-polarization of the backfolded Mahan cones for monolayer films of CuPc and H2Pc on Au(111). For both molecular adsorbates, we observe a clear spin-polarization for the main Mahan cones, but not for the backfolded cones. A comparison of our results with previous findings for the Mahan cone spin polarization for the bare Au(111) surface and Bi/Au(111) interfaces will allow us to gain insight into spin-dependent scattering and spin-dependent back-folding of substrate bands at adsorbate films.

O 90.2 Thu 10:45 MA 042

**Manipulating electron scattering resonances in graphene** — ●MAXIM KRIVENKOV, DMITRY MARCHENKO, JAIME SÁNCHEZ-BARRIGA, OLIVER RADER, and ANDREI VARYKHALOV — Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

Scattering resonances were recently predicted to exist above the vacuum level of two-dimensional (2D) materials [1]. These resonances influence transmission of low-energetic electrons and should appear in photoemission experiments as strongly dispersive features of suppressed intensity. We were able to observe and systematically study these states in graphene by using angle-resolved photoemission spectroscopy. To investigate whether the resonances can be manipulated we explored three routes: growth of graphene on chemically diverse substrates - Ir(111), Bi/Ir, and Ni(111), enhancement of superlattice potential by Ir nanodots [2] and switching of hybridization type in graphene from  $sp^2$  to  $sp^3$  by hydrogenation. While strength of the chemical interaction with the substrate had almost no effect on the dispersion of the resonances, their energy varies with the magnitude of charge transfer from/to graphene. In contrast, deposition of superlattice of Ir nanodots as well as hydrogenation of graphene eliminate the resonances completely. Our results provide the ways of tuning optoelectronic properties of 2D materials with a graphene-like structure.

[1] V. U. Nazarov et al., Phys. Rev. B 87, 041405(R) (2013);

[2] M. Krivenkov et al., Appl. Phys. Lett. 111, 161605 (2017).

O 90.3 Thu 11:00 MA 042

**The nature of surface conductivity in samarium hexaboride** — PETER HLAWENKA<sup>1</sup>, KONRAD SIEMENSMEYER<sup>1</sup>, EUGEN WESCHKE<sup>1</sup>, JAIME SÁNCHEZ-BARRIGA<sup>1</sup>, ANDREI VARYKHALOV<sup>1</sup>, NATALYA SHITSEVALOVA<sup>2</sup>, SLAVOMIR GABÁNI<sup>3</sup>, KAROL FLACHBART<sup>3</sup>, OLIVER RADER<sup>1</sup>, and ●EMILE RIENKS<sup>4,5</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Berlin, Germany — <sup>2</sup>National Academy of Sciences of Ukraine, Kiev, Ukraine — <sup>3</sup>Slovak Academy of Sciences, Košice, Slovakia — <sup>4</sup>Technische Universität Dresden, Dresden, Germany — <sup>5</sup>IFW Dresden, Dresden, Germany

The prediction that Kondo insulators could be topologically non-trivial renewed interest in SmB<sub>6</sub>, a material that already earned a reputation as the first mixed valence system and Kondo insulator. Dzero et al.'s proposal [1] connects two of the most topical fields in solid state research: Topological insulators and strongly correlated materials. In addition, robust surface conductivity—inherent to a topological insulator—would elegantly explain SmB<sub>6</sub>'s anomalous transport properties. The notion that samarium hexaboride is a topological Kondo insulator is seemingly confirmed by recent experiments: It is found to be a surface-only conductor at low temperature and surface states have been found at the expected locations [2]. In this talk we will present crucial new insights from high-resolution angle-resolved photoemission spectroscopy [3] and discuss the implications.

[1] M. Dzero, et al., Phys. Rev. Lett., 104 (2010) 106408. [2] J. W. Allen, Phil. Mag. 96 (2016) 3227. [3] First results: P. Hlawenka et al.,

ArXiv: 1502.01542v1.

O 90.4 Thu 11:15 MA 042

**Spin-polarization of the two-dimensional electron gas at CaTiO<sub>3</sub> film surfaces** — ●EDUARDO B. GUEDES<sup>1,2</sup>, STEFAN MUFF<sup>1,2</sup>, MILAN RADOVIC<sup>2,3</sup>, and J. HUGO DIL<sup>1,3</sup> — <sup>1</sup>Institut de Physique, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland — <sup>2</sup>Swiss Light Source, Paul Scherrer Institut, 5232 Villigen, Switzerland — <sup>3</sup>SwissFel, Paul Scherrer Institut, 5232 Villigen, Switzerland

The perovskite CaTiO<sub>3</sub> was recently added to the group of oxides hosting a metallic surface state [1], which in this case consists exclusively of 2-dimensional electron gas (2DEG). We investigated films of CaTiO<sub>3</sub> grown by pulsed laser deposition by means of spin- and angle-resolved photoelectron spectroscopy (SARPES). Our results show that the surface state is clearly split into two bands, which present spin polarization consistent with a Rashba-like splitting. Further, possible spin-interference effects [2] are also seen in the spectra, and different scenarios for the role of spin in dipole selection rules will be discussed.

**References:**[1] S. Muff et al., Observation of a two-dimensional electron gas at CaTiO<sub>3</sub> film surfaces, Appl. Surf. Sci. (2017), <http://dx.doi.org/10.1016/j.apsusc.2017.05.229>.

[2] U. Heinzmann and J. H. Dil, J. Phys.: Condens. Matter 24, 173001 (2012).

O 90.5 Thu 11:30 MA 042

**Origin of Surface States in ZrSiS and related compounds** — ●ANDREAS TOPP<sup>1</sup>, RAQUEL QUEIROZ<sup>1,2</sup>, LESLIE M. SCHOOP<sup>1,3</sup>, and CHRISTIAN R. AST<sup>1</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Stuttgart, DEU-70569 — <sup>2</sup>Weizmann Institute of Science, Rehovot, ISR-7610001 — <sup>3</sup>Department of Chemistry, Princeton University, Princeton, USA-08544

Three-dimensional Dirac semimetals, which accommodate massless Dirac and Weyl fermions, show exotic physical properties, e.g. an extremely high mobility and giant magnetoresistance. Compounds that comprise nonsymmorphic symmetries are especially interesting as the band crossings that are protected by the symmetry, are not affected by SOC. ZrSiS, hosting a square lattice of Si atoms, has shown normal, as well as, nonsymmorphically protected 3D Dirac crossings at and close to the Fermi level [1]. ARPES measurements showed additional surface states crossing the bulk bands, which do not fit in the current scheme of surface states. Here, we analyze their origin by comparing ARPES data with DFT and tight-binding calculations. We present the idea of a selective symmetry breaking through the surface that lifts the nonsymmorphic degeneracy at the X point and leads to the formation of these surface states.

[1] L. M. Schoop et al., Nat. Comm. 7, 11696 (2016).

O 90.6 Thu 11:45 MA 042

**Manipulation of the 2DEG at Titanates Surfaces** — ●STEFAN MUFF<sup>1,2</sup>, NICOLAS PILET<sup>2</sup>, MAURO FANCIULLI<sup>1,2</sup>, ANDREW P. WEBER<sup>1,2</sup>, ZORAN RISTIC<sup>2</sup>, ZHIMING WANG<sup>2,3</sup>, EDUARDO BONINI GUEDES<sup>1,2</sup>, NICHOLAS PLUMB<sup>2</sup>, MILAN RADOVIC<sup>2</sup>, and HUGO DIL<sup>1,2</sup> — <sup>1</sup>Institut de Physique, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne — <sup>2</sup>Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen — <sup>3</sup>Department of Quantum Matter Physics, University of Geneva, CH-1211 Geneva

In this talk, different ways to manipulate the 2DEG of the titanates (001) surface are presented. Crystalline surfaces and films grown by pulsed laser deposition (PLD) are studied by the help of angle-resolved photoelectron spectroscopy (ARPES) to explore the changes in the orbital ordering and band filling of the studied compounds.

In vicinal SrTiO<sub>3</sub> and films of CaTiO<sub>3</sub>, the tetragonal distortion of the TiO<sub>6</sub> octahedra is altered due to the changed surface free energy and chemical strain respectively. With the strong dependence of the formation of the titanates 2DEG on the surface crystal structure, the change in distortion directly affects the energy scale of the orbital ordering of the Ti 3d states, that form the 2DEG of these two systems. For thin films of SrTiO<sub>3</sub> grown by PLD, the different type of growth defects and the surface potential landscape are responsible for an observed change in band filling of the 2DEG. The presented results

show different ways to manipulate the 2DEG of titanates surfaces and open new paths to engineer the 2DEG and consequently the transport properties of the studied and closely related systems.

O 90.7 Thu 12:00 MA 042

**Electronic structure of the non-polar GaN(10 $\bar{1}$ 0) surface** — MARTIN FRANZ<sup>1</sup>, STEPHAN APPELFELLER<sup>1</sup>, HOLGER EISELE<sup>1</sup>, PHILIPP EBERT<sup>2</sup>, and MARIO DÄHNE<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Technische Universität Berlin — <sup>2</sup>Peter Grünberg Institut, Forschungszentrum Jülich

The non-polar GaN(10 $\bar{1}$ 0) surface, the so-called m-plane, plays an important role in nitride devices, e.g. as the predominant sidewall facet of nanowires or as a promising growth substrate for a reduction of polarization fields. However, detailed experimental results on the nature of the GaN(10 $\bar{1}$ 0) surface states are still scarce.

In this work, the electronic structure of the *n*-GaN(10 $\bar{1}$ 0) cleavage surface was studied using angle-resolved photoelectron spectroscopy at BESSY. The bulk valence bands and the filled nitrogen-related surface-state band could be clearly identified, allowing to determine the dispersion of the surface-state band and to derive the effective masses for both the bulk and surface valence bands. In addition, the position of the Fermi level within the band gap was determined at around 2.3 eV above the valence-band maximum, corresponding to the energetic position of the minimum of the empty gallium-related surface-state band, in nice agreement with recent theoretical results [1].

This work was supported by the DFG, Sfb 787, TP A4.

[1] L. Lymperakis, P.H. Weidlich, H. Eisele, M. Schnedler, J.-P. Nys, B. Grandier, D. Stiévenard, R.E. Dunin-Borkowski, J. Neugebauer, and P. Ebert, *Appl. Phys. Lett.* **103**, 152101 (2013).

O 90.8 Thu 12:15 MA 042

**Observation of a remarkable reduction of correlation effects in BaCr<sub>2</sub>As<sub>2</sub> by ARPES** — JAYITA NAYAK<sup>1</sup>, KAI FILSINGER<sup>1</sup>, GERHARD H. FECHER<sup>1</sup>, STANISLAV CHADOV<sup>1</sup>, JAN MINÁR<sup>2</sup>, EMILE D. L. RIENKS<sup>3,4</sup>, BERND BUCHNER<sup>3,4</sup>, JORG FINK<sup>1,3</sup>, and CLAUDIA FELSER<sup>1</sup> — <sup>1</sup>Max Planck Institute CPFS, Dresden, Germany — <sup>2</sup>University of West Bohemia, Pilsen, Czech Republic — <sup>3</sup>Institute for Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden, D- 01171 Dresden, Germany — <sup>4</sup>Institute for Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden, D- 01171 Dresden, Germany

The superconducting phase in iron-based high-T<sub>c</sub> superconductors (FeSC) neighbors a magnetically ordered one in the phase diagram. This proximity hints at the importance of electron correlation effects in these materials. Hund's exchange interaction has been suggested to be the dominant correlation effect in FeSCs because of their multi-band nature. Correlation should be strongest for materials closest to a half filled 3d electron shell (Mn compounds, hole-doped FeSCs) and decrease for systems with both higher (electron-doped FeSCs) and lower (Cr-pnictides) 3d counts. Here we find that the strength of correlation effects in nonsuperconducting antiferromagnetic BaCr<sub>2</sub>As<sub>2</sub> is strongly reduced. We have used angle-resolved photoemission spectroscopy (ARPES) and first-principles calculations for this investiga-

tion.

O 90.9 Thu 12:30 MA 042

**The XPS limit within the one-step model of photoemission: an application to Ag(100)** — LAURENT NICOLAI<sup>1</sup>, VLADIMIR STROCOV<sup>3</sup>, JURAJ KREMPASKÝ<sup>3</sup>, HUBERT EBERT<sup>2</sup>, JÜRGEN BRAUN<sup>2</sup>, FEDERICO BISTI<sup>3</sup>, and JÁN MINÁR<sup>1</sup> — <sup>1</sup>University of West Bohemia, Plzeň, Czech Republic — <sup>2</sup>Ludwig-Maximilians-Universität Munich, Germany — <sup>3</sup>Paul Scherrer Institut, Villigen, Suisse

Angle-Resolved Photoemission Spectroscopy (ARPES) is the method of choice for characterising the electronic structure of a given crystalline material. Within the Ultra-Violet (UV) regime, theory can nicely reproduce experimental spectra using the k-conserving dipole selection rules within the one-step model of photoemission [1,2]. Yet, this model is no longer sufficient when dealing with the soft/hard X-ray or high temperature regimes: the XPS-limit. For this case, one has phonon-assisted electronic transitions such that the dipole selection rules cannot describe by themselves the experimentally obtained spectra [3]. Here we use the so-called alloy analogy model in order to quantify the importance of non-dipole transitions. This rather new model is here tested by comparison to new experimental data obtained for the Ag(100) system. [1] J. Braun, *Rep. Prog. Phys.* **59**, 1267-1338 (1996), [2] H. Ebert, D. Ködderitzsch and J. Minár, *Rep. on Prog. in Phys.* **74**, 096501 (2011), [3] J. Braun et al., *Phys. Rev. B* **88**, 205409 (2013)

O 90.10 Thu 12:45 MA 042

**The 3D electronic structure of Os(0001) and Re(0001) probed by angle- and spin-resolved soft x-ray photoemission** — CHRISTIAN MENDE<sup>1</sup>, JÜRGEN BRAUN<sup>1</sup>, JAN MINÁR<sup>2</sup>, HANS-JOACHIM ELMERS<sup>3</sup>, Gerd SCHÖNHENSE<sup>3</sup>, and HUBERT EBERT<sup>1</sup> — <sup>1</sup>Dept. Chemie, LMU München, Germany — <sup>2</sup>NTRC, University of West Bohemia, Plzeň, Czech Republic — <sup>3</sup>Institut für Physik, JGU Mainz, Germany

In this contribution we discuss the impact of the spin-orbit coupling on the 3D electronic structure of hcp Os(0001) and Re(0001) as reflected by angle- and spin-resolved soft x-ray photoemission. The spectroscopical analysis has been performed within the framework of the fully relativistic version of the one-step model of photoemission in its spin-density matrix formulation [1]. For this purpose the underlying electronic structure is calculated self-consistently for a semi-infinite half-space configuration using the so called tight-binding (TB) mode of the KKR (Korringa-Kohn-Rostoker) method [2]. To guarantee for a quantitative description of the surface-sensitive spectral features special attention is paid to the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism. The results that give clear evidence for a pronounced impact of spin-orbit coupling will be discussed in detail in comparison with recent experimental work.

[1] J. Braun et al., *New Journal of Physics* **16**, 015005 (2014).

[2] H. Ebert et al., The Munich SPR-KKR package, version 7.7.0, <http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR> (2017).