

## O 46: Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:30–20:30

Location: P1A

O 46.1 Tue 18:30 P1A

**Influence of the Surface Structure on Photoelectron Momentum Maps Measured for Coronene Monolayers on Ag(111)** —

•CHRISTIAN UDHARDT<sup>1</sup>, FELIX OTTO<sup>1</sup>, TINO KIRCHHÜBEL<sup>1</sup>, FALKO SOJKA<sup>1</sup>, TOBIAS HÜMPFNER<sup>1</sup>, MATTHIAS MEISSNER<sup>1</sup>, CHRISTIAN KERN<sup>2</sup>, DANIEL LÜFTNER<sup>2</sup>, PETER PUSCHNIG<sup>2</sup>, BERND SCHRÖTER<sup>1</sup>, ROMAN FORKER<sup>1</sup>, and TORSTEN FRITZ<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — <sup>2</sup>Institute of Physics, University of Graz, 8010 Graz, Austria

Photoelectron momentum maps (PMMs) can be helpful to investigate molecular states near the Fermi edge, even though their discussion may be complicated by substrate- and film-induced effects. Here, we present PMMs of 1 ML coronene thin films on Ag(111) and compare them to simulations of a free coronene molecule, the  $4 \times 4$  film structure observed with low-energy electron diffraction (LEED), and angle-resolved ultraviolet photoemission spectroscopy (ARUPS). While the substructure observed in the PMM of the highest occupied molecular orbital (HOMO) is shown to coincide with the structure of the coronene film, the features in the PMM taken at the Fermi edge are conform with a film-induced back-folding of substrate bands without the influence of a molecular state.

O 46.2 Tue 18:30 P1A

**STM-Investigations of  $\kappa$ -(BEDT-TTF)<sub>2</sub>X-Charge Transfer Salts** — •TORGE MASHOFF, JOHANNES REGEL, and HANS-JOACHIM ELMERS — Institut für Physik, Johannes Gutenberg-Universität, Mainz

Organic charge-transfer salts of the  $\kappa$ -(BEDT-TTF)<sub>2</sub>X family offer exciting many-body physics manifesting in an interesting phase diagram with a neighboring superconducting and Mott insulating phase. This results in a strong deviation of the superconducting properties from BCS theory and has been attributed to their two-dimensional structure leading to electronic correlation effects. We investigated small crystals of the two charge-transfer salts  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br and  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> using a low temperature scanning tunneling microscope and obtained good topographic resolution of the crystallographic structure. Both crystals show similar crystallographic order but due to the higher chemical pressure of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>, they have different positions in the phase diagram. We used scanning tunneling spectroscopy to investigate the electronic properties and the influence of the proximity to the Mott phase.

O 46.3 Tue 18:30 P1A

**Time-resolved momentum microscopy with fs-XUV light**

— •CHRISTINA SCHOTT<sup>1</sup>, MARKUS ROLLINGER<sup>1</sup>, SEBASTIAN EMMERICH<sup>1</sup>, JOHANNES SEIDEL<sup>1</sup>, FLORIAN HAAG<sup>1</sup>, NORMAN HAAG<sup>1</sup>, STEFFEN EICH<sup>1</sup>, MIRKO CINCHETTI<sup>2</sup>, BENJAMIN STADTMÜLLER<sup>1</sup>, and MARTIN AESCHLIMANN<sup>1</sup> — <sup>1</sup>University of Kaiserslautern and Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — <sup>2</sup>Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Time resolved photoemission spectroscopy with a fs-XUV light source is a powerful technique to investigate ultrafast optically induced electron dynamics in solid state systems [1,2]. The combination of this technique with momentum microscopy, a novel tool for angle resolved photoemission, allows us to capture transient snapshots of the ultrafast dynamics for both parallel momentum components for one fixed binding energy. Together with the large photon energy of our fs-XUV light source, we can access the electron dynamics throughout the entire first Brillouin zone of typical sample systems. Here, we will show the capability of our new setup for time-resolved optical-pump, fs-XUV probe momentum microscopy. We will discuss experimental challenges such as space charge effects and long-term stability using dedicated sample systems. Moreover, we will present our first results of the transient band structure dynamics of metallic surfaces using time-resolved momentum microscopy.

[1] Rohwer et al, Nature (2011) [2] Eich et al, J. el. Spec (2014)

O 46.4 Tue 18:30 P1A

**Spin-polarized surface states of Pb monolayers on Si(111)** —

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Atomic monolayers (ML) of Pb/Si(111) have recently been found to be superconducting below  $T_C \approx 1.8$  K, but the mechanism behind the evolution of these 2d states is not understood yet. In the range from 6/5 ML to 4/3 ML supercells consisting of linear combinations of  $(\sqrt{7} \times \sqrt{3})$  and  $(\sqrt{3} \times \sqrt{3})$  unit cells are formed (so-called Devil's staircase regime). This allows us to tune the spin-orbit interaction (SOI), the electronic and atomic structure via adsorption of minute amounts of Pb. In this study we present STM and (SR)-ARPES measurements at low  $T$  ( $> T_C$ ) to evaluate the influence of the SOI on the Pb surface states. As it turns out the local adsorption geometry and symmetry of the atomic structure plays an important role for the understanding of the measured spin-polarization by SR-ARPES showing strongly spin-polarized metallic surface states. The experimental results are in very good agreement with DFT calculations and reveal beside a complex spin-texture at  $E_F$  large Rashba- and Zeeman-type spin-splittings of the Pb surface states.

O 46.5 Tue 18:30 P1A

**2D Dirac cones at the Fermi level in ZrSiTe** — •SHWETA SHEORAN<sup>1</sup>, ANDREAS TOPP<sup>1</sup>, JUDITH M. LIPPMANN<sup>1,2</sup>, ANDREI VARYKHALOV<sup>3</sup>, VIOLA DUPPEL<sup>1</sup>, BETTINA V. LOTSCH<sup>1,2,4</sup>, CHRISTIAN R. AST<sup>1</sup>, and LESLIE M. SCHOOP<sup>1</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, D-70569 Stuttgart — <sup>2</sup>Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — <sup>3</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, D-12489 Berlin — <sup>4</sup>Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-80799 München

A new class of materials exhibiting non-symmorphic symmetry has generated great interest, due to the associated rich physics such as ultra high mobility, giant magneto-resistance and also it's essential role in the discovery of new quasi particles beyond the usual Dirac, Weyl and Majorana fermions. Experimental analysis shows that the material ZrSiS, exhibits Dirac cones protected by non-symmorphic symmetry below the Fermi level [1]. A major requirement for pinning these non-symmorphic crossings at the Fermi level is a half filled band, which is quite difficult to achieve. A possible workaround could be the application of uniaxial tensile strain. In ZrSiS, this would be equivalent to substitution of S by Te, leading to the isostructural and isoelectronic compound ZrSiTe. Here we present the DFT bandstructure calculations and ARPES measurements performed on ZrSiTe, showing that it exhibits a Dirac line node on the Fermi level.

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

O 46.6 Tue 18:30 P1A

**Multi-electron photon-emission from a tunnel junction** —

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Inelastic tunneling processes in the tip/sample junction of a scanning tunneling microscope (STM) can excite tip induced plasmon modes (TIP), which can decay radiatively. The emitted light carries information about the underlying inelastic processes. We observe light emission between the visible and the near infrared range from the junction between a silver covered STM tip and a Ag(111) surface. The applied voltage  $V_{Bias}$ , limits the maximum energy  $E_{max} = eV_{Bias}$  of the tunneling electrons. Normalized Emission spectra show emission tails exceeding  $E_{max}$ , supposedly caused by natural linewidth broadening. A comparison with calculated tunneling probabilities for inelastic transitions results in electron-lifetimes of the excited states in the range of 30 fs to 80 fs. If the tunneling current  $I_T$  is unusual high (nA to  $\mu$ A), two or more electrons may interact and exchange energy and non-linear processes may be triggered [1], [2]. In this case, photons with an energy  $E_{max} < E_{photon} < 2E_{max}$  can be observed. For these cases, spectra of emitted light are discussed as a function of the tunneling parameters. However, the emission spectra reveal the same spectral

features, indicating that the same TIP modes are excited.

- [1] G. Hoffmann et al., Phys. Rev. Lett. 90, 046803-1 (2003).  
 [2] G. Schull et al., Phys. Rev. Lett. 102, 057401 (2009).

O 46.7 Tue 18:30 P1A

**Investigation of charge puddles at the surface of the compensated topological insulator BiSbTeSe<sub>2</sub>** — ●TIMO KNISPTEL, WOUTER JOLIE, NICK BORGHARDT, ZHIWEI WANG, JONATHAN LUX, ACHIM ROSCH, YOICHI ANDO, MARKUS GRÜNINGER, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln, Germany

BiSbTeSe<sub>2</sub> is a three dimensional topological insulator which is characterized by an insulating bulk state and a gapless Dirac cone at the  $\Gamma$ -point, with the chemical potential near the Dirac point [1]. Large fluctuations in the Coulomb potential of the dopants cause self-organized charge puddles in the bulk, which in turn cause substantial rigid shifts of the local bulk band structure. Surprisingly, these charge puddles evaporate around 50 K [2]. Here we investigate by STM and STS charge puddles at the surface of BiSbTeSe<sub>2</sub> and how they are linked to the bulk ones.

In atomic resolution STM and STS measured over a broad energy range we identify (i) a short length scale due to variations in chemical composition, (ii) a medium energy-dependent length scale due to quasi-particle scattering, and (iii) a large length scale which we attribute to surface charge puddles. By point spectroscopy we measure Dirac point fluctuations of  $\Delta E = 25$  meV around an average of +30 meV. Through temperature dependent experiments we analyze the coupling of the surface charge puddles to their bulk counterparts.

- [1] T. Arkane et al., Nat. Comm. 3, 636 (2012)  
 [2] N. Borgwardt et al., Phys. Rev. B 93, 245149 (2016)

O 46.8 Tue 18:30 P1A

**Studying the type-II Weyl semimetal Td-WTe<sub>2</sub> with two-photon photoemission** — ●PETRA HEIN<sup>1</sup>, STEPHAN JAUERNIK<sup>1</sup>, YULIN CHEN<sup>2</sup>, LEXIAN YANG<sup>2</sup>, BINGHAI YAN<sup>3</sup>, CLAUDIA FELSER<sup>3</sup>, and MICHAEL BAUER<sup>1</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, University of Kiel, Germany — <sup>2</sup>Physics Department, Tsinghua University, Beijing, China — <sup>3</sup>Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

With their first experimental observation in 2015, topological Weyl semimetals have attracted enormous attention: In these materials, the long sought-after Weyl fermions are realized as quasi-particle excitations in condensed matter [1]. Weyl semimetals feature an unusual electronic structure with touching points in the bulk band structure – the so-called Weyl points – that are connected by unique topological surface Fermi arcs. The key technique to gain access to these signatures is angle-resolved photoelectron spectroscopy (ARPES) [2,3].

Here, we present a combined photoemission and two-photon photoemission (2PPE) study of the type-II Weyl semimetal Td-WTe<sub>2</sub>. Using a widely tunable femtosecond laser system with photon energies between 1.3 eV and 5.0 eV, we are able to access a variety of both occupied and unoccupied electronic states. The results are discussed under consideration of band structure calculations and current ARPES studies of Td-WTe<sub>2</sub>.

- [1] A. Vishwanath, Physics 8, 84 (2015).  
 [2] S.-Y. Xu et al., Science 349, 6248 (2015).  
 [3] Y. Wu et al., Phys. Rev. B 94, 121113(R) (2016).

O 46.9 Tue 18:30 P1A

**Thickness-dependent photoelectron spectroscopy study of 1,2,8,9-dibenzopentacene on Au(111)** — ●MAXIMILIAN SCHAAL, FELIX OTTO, CHRISTIAN UDHARDT, BERND SCHRÖTER, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Alkali-metal-doped polycyclic aromatic hydrocarbons received broad attention as potential organic superconductors during the last years. A representative of this class is potassium-doped 1,2,8,9-dibenzopentacene (DBPen) which has a reported transition temperature of 33 K in bulk powder samples [1]. Here we investigate thin films of DBPen on Au(111) by means of thickness-dependent x-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). The XPS results show a thickness-independent line shape and an energy shift by the formation of an interface dipole. The UPS results show an asymmetric broadening of the highest occupied molecular orbital (HOMO) in the monolayer which is attributed to the occurrence of vibronic states. The HOMO splitting in the bilayer indicates the formation of a dimer structure via  $\pi$ -stacking. Furthermore, we explore

the thickness-dependent modification of the binding energy and effective mass of the Shockley surface state of Au(111) by angle-resolved UPS (ARUPS).

- [1] M. Xue et al., Sci. Rep. 2, 389 (2012).

O 46.10 Tue 18:30 P1A

**Electronic Properties of Coronene on (111)-Surfaces of the Coinage Metals.** — ●CHRISTIAN SIMON KERN<sup>1</sup>, DANIEL LÜFTNER<sup>1</sup>, CHRISTIAN UDHARDT<sup>2</sup>, FELIX OTTO<sup>2</sup>, ROMAN FORKER<sup>2</sup>, TORSTEN FRITZ<sup>2</sup>, and PETER PUSCHNIG<sup>1</sup> — <sup>1</sup>University of Graz, Institute of Physics, NAWI Graz - Universitätsplatz 5, A-8010 Graz, Austria — <sup>2</sup>Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena, Germany

Mono-layers of the polycyclic aromatic hydrocarbon coronene adsorbed on (111)-surfaces of the metals copper, silver and gold are investigated by density functional theory.

First, we have determined the most favorable adsorption sites and molecular orientations based on the experimentally known over-layer structures. Particularly, for Ag(111) we find a flat adsorption geometry with an azimuthal orientation in good agreement with the experimental orientation. In a second step, we have simulated angle-resolved photoemission spectroscopy (ARPES) experiments for coronene on the three coinage metal (111)-surfaces, focusing on the emission from the HOMO. Simulated photoelectron angular distributions (PADs) for the coronene/metal interface show pronounced differences to PADs of the two-fold degenerate HOMO of the isolated molecule. We conclude that the observed symmetry-breaking results from the molecule-substrate-interaction and intermolecular band dispersion. The observed substructure of the major emission features in the PADs compares well to the experimental findings.

O 46.11 Tue 18:30 P1A

**Charge-ordered state in the low-temperature phase of Pb/Si(111)** — ●FLORIAN ADLER<sup>1</sup>, MANUEL LAUBACH<sup>2</sup>, STEPHAN RACHEL<sup>2</sup>, JÖRG SCHÄFER<sup>1</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikalisches Institut und Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — <sup>2</sup>Institut für Theoretische Physik, Technische Universität Dresden, Germany

Two-dimensional triangular lattices of Group IV adatoms on diamond lattice substrates provide a rich playground for experimental studies and many-body calculation techniques. For the system investigated in this work, 1/3 monolayer of Pb on Si(111), preceding studies have noted a phase transition from  $\sqrt{3} \times \sqrt{3}$  to  $3 \times 3$  at 86 K. In our high-resolution scanning tunneling microscopy and spectroscopy measurements in the low-temperature phase, we have unveiled the formation of a charge-ordered state by carefully mapping the local density of states. Furthermore, we find a structural rearrangement with a 2-up/1-down configuration. These results are supported by state-of-the-art many body calculations using the Variational Cluster Approach (VCA), which is sensitive to both spin- and charge-density wave instabilities. I will present a comparison of our measurements and the latest results from VCA calculations.

O 46.12 Tue 18:30 P1A

**A new dual analyzer system for surface analysis of liquids under UHV conditions** — ●FRANCESCO GRECO, INGA NIEDERMAIER, CLAUDIA KOLBECK, HANS-PETER STEINRÜCK, and FLORIAN MAIER — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In the last decade, ionic liquid (IL) systems have emerged for UHV studies of liquid surfaces and interfaces due to the extremely low IL vapor pressure. It has been demonstrated that particularly angle-resolved X-ray Photoelectron Spectroscopy (ARXPS) allows for investigating phenomena that occur at gas-liquid and liquid-solid interfaces on the molecular level. In all of these ARXPS studies, the sample holder had to be tilted in order to change the polar detection angle of the emitted photoelectrons, which restricted the investigations to very thin and high-viscous IL films only. We here report on a new and unique laboratory "Dual Analyzer System for Surface Analysis (DASSA)" which enables fast ARXPS, UV photoelectron spectroscopy, imaging XPS, and low-energy ion scattering of macroscopically thick non-volatile liquid samples.[1] As core element, it comprises a UHV analysis chamber equipped with two electron analyzers mounted for simultaneous measurements in 0° and 80° emission relative to the surface normal for horizontally mounted IL samples.

F.G. and H.P.S. thank the ERC for financial support through an Advanced Investigator Grant to H.P.S.!

[1] I. Niedermaier, C. Kolbeck, H.-P. Steinrück, F. Maier, Rev. Sci. Instrum. 87 (2016) 045105

O 46.13 Tue 18:30 P1A

**Quasiparticle interferences in highly doped bilayer graphene** — ●WOUTER JOLIE<sup>1</sup>, JONATHAN LUX<sup>2</sup>, MATHIAS PÖRTNER<sup>1</sup>, TOBIAS HARTL<sup>1</sup>, TIMO KNISPEL<sup>1</sup>, SABINA SIMON<sup>1,3</sup>, CHARLOTTE HERBIG<sup>1</sup>, THOMAS MICHELY<sup>1</sup>, and CARSTEN BUSSE<sup>1,4</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln — <sup>2</sup>Institut für Theoretische Physik, Universität zu Köln — <sup>3</sup>Fachbereich Physik, Universität Konstanz — <sup>4</sup>Institut für Materialphysik, Universität Münster

When two graphene layers are Bernal stacked as in graphite, the two low-energy bands can be described by massive Dirac fermions and it has been demonstrated that doping such a graphene bilayer not only shifts its chemical potential, but also opens up a band gap [1]. We dope bilayer graphene to populate the second conduction band and measure quasiparticle interferences (QPI) with scanning tunneling microscopy and spectroscopy.

We grow bilayer graphene on Ir(111) with a combination of chemical vapor deposition (creating a monolayer of high perfection) and physical vapor deposition (forming a second graphene layer at the interface). Subsequently, Cs is intercalated between the bilayer and the metal underneath.

We observe complex standing waves patterns at various energies and obtain the scattering vectors responsible for QPI using a Fourier transform analysis. We compare our results with simulations based on the  $T$ -matrix theory as well as tight-binding calculations and explore the origin of the suppression of certain scattering processes.

[1] E. V. Castro et al., Phys. Rev. Lett. 99, 216802 (2007)

O 46.14 Tue 18:30 P1A

**Systematics of 3d transition metal-doped  $\text{Sb}_2\text{Te}_3$**  — ●JOHANNES JUNG, THOMAS BATHON, PAOLO SESSI, and MATTHIAS BODE — Universität Würzburg; Physikalisches Institut; Experimentelle Physik II, Würzburg, Germany

Time-reversal symmetry plays a crucial role in topological insulators (TIs). Once broken, topological surface states become gapped and unconventional states of matter such as the quantum anomalous Hall effect can be realized.

Here, we present a systematic investigation of the prototypical TI  $\text{Sb}_2\text{Te}_3$  where different magnetic perturbations are introduced by bulk-doping with 3d transition elements (V, Cr, Mn, Fe). The dopants adsorption sites are localized and classified by atomically resolved scanning tunneling microscopy, while scanning tunneling spectroscopy allows to visualize their influence on the local electronic environment of the host material.

[1] P. Sessi *et al.*, Nature Communications, 7, 12027 (2016).

O 46.15 Tue 18:30 P1A

**New insights into the LaB6 (001)-surface obtained by Scanning Tunneling Microscopy** — ●PHILIPP BUCHSTEINER<sup>1</sup>, MARTIN WENDEROTH<sup>1</sup>, and GEETHA BALAKRISHNAN<sup>2</sup> — <sup>1</sup>IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — <sup>2</sup>Department of Physics, University of Warwick, United Kingdom

Lanthanum Hexaboride (LaB6) has attracted much attention due to its surface properties, such as an unusually low work function [1]. However, up to now only few investigations of the (001)-surface of single crystalline LaB6 using Scanning Tunneling Microscopy (STM) have been performed [2]. Our STM findings of that surface have led to striking differences for the surface structure: firstly, we have not observed any vacancies at the surface, which we relate to our different sample preparation by cleavage. Secondly, we have observed a long range height modulation within atomically resolved constant current topographies. We are hypothesizing that the modulation is caused by single interstitial and vacant boron atoms within the hexaboride lattice. Such imperfections are probably generated during crystal growth, since the B/La ratio deviates slightly in the bulk material for most crystals from 6.00 [3]. [1] M. Trenary, Sci. Technol. Adv. Mater. 13 (2012), [2] J.S. Ozcomert, M. Trenary, Surf. Sci., 265 (1992), [3] T. Tanaka, S. Otani, Prog. Cryst. Growth Charact. Mater. 16 (1988)

O 46.16 Tue 18:30 P1A

**Preparation and Characterization of Sub-Monolayer Ge on Cu** — ●THOMAS KOTZOTT, WEI LI, and MARTIN WENDEROTH — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Semiconductor growth on metals is of interest for designing and producing devices in semiconductor-based electronics. In this study, we have prepared different copper-germanium surface structures. Clean Cu single crystal surfaces are fabricated by sputtering and annealing and characterized by LEED and AES. Sub-monolayer Ge is deposited at 100K using electron beam evaporators in-situ under UHV conditions at a base pressure of  $p < 10^{-10}$  mbar. The Ge/Cu surfaces are investigated by low temperature (6K) scanning tunneling microscopy. We present topography data and the corresponding electronic structure obtained by scanning tunneling spectroscopy as well as thermovoltage measurements. The scattering processes at the Cu surface are examined, finally aiming for the scattering properties of a single semiconductor impurity within the bulk metal using dilute alloys.

O 46.17 Tue 18:30 P1A

**Polarization-dependent two-photon photoemission from p-doped topological insulators  $\text{SnBi}_x\text{Sb}_{2-x}\text{Te}_4$  and  $\text{GeSb}_2\text{Te}_4$**  — ●SEBASTIAN OTTO, JONAS RIETSCH, PHILIPP ROSENZWEIG, DANIEL NIESNER, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

Polarization-dependent, time- and angle-resolved two-photon photoemission is used to study the electronic structure of septuple-layered antimony telluride crystals of different p-dopings. All surfaces show a linearly dispersing surface state bridging the band gap with a Dirac point at  $E_F + 0.42 \pm 0.05$  eV for  $\text{GeSb}_2\text{Te}_4$  and  $E_F + 0.31 \pm 0.02$  eV for the  $\text{SnBi}_x\text{Sb}_{2-x}\text{Te}_4$  crystals. The Bi-doping of the  $\text{SnBi}_x\text{Sb}_{2-x}\text{Te}_4$  (with  $x = 0, 0.1, 0.2$ ) causes no shift of the energetic position of the Dirac point, but a decrease in group velocity which is reflected in the dynamics of the systems. The lifetimes of the topological surface states range from  $10 \pm 5$  fs to  $120 \pm 20$  fs and time constants of the conduction band minimum are found between  $180 \pm 10$  fs and  $300 \pm 20$  fs. Measurements with circularly polarized probe pulses verify the topological nature of the surface states. The excitation of the topological surface state shows no dependence on the polarization of the pump pulse.

O 46.18 Tue 18:30 P1A

**Characterisation of Beryllides with XPS** — ●NICOLA HELFER, PETRA HANSEN, HANS RUDOLF KOSLOWSKI, and CHRISTIAN LINSMEIER — Forschungszentrum Jülich GmbH, Institut für Energie und Klimaforschung – Plasmaphysik, 52425 Jülich

Future fusion reactors need to produce their tritium fuel. A self-sustained fuel cycle requires a neutron multiplier material, e.g. Be, within the breeding blanket. Beryllides are promising materials since their chemical reactivity with structural material is lower than for pure Beryllium [Y. Mishima et al., J. Nucl. Mat. 367–370, 1382 (2007)]. Beside the production process, the thermal stability and phase transitions are of great interest.

Be-metal alloy samples, produced by Wright Air Development Center already in 1959 were available for experimental investigation. The characterisation of the thermal stability of  $\text{Be}_{12}\text{Ta}$  and  $\text{Be}_{12}\text{Ti}$  with x-ray photoelectron spectroscopy (XPS) is presented here. X-ray diffraction measurements are utilised to confirm the crystalline phase of the samples.

Binding energy shifts of the Be 1s states have been observed and are compared to recent Density Functional Theory (DFT) simulations with an all-electron code (FLEUR) [J. Bröder, master thesis, RWTH Aachen 2015].

O 46.19 Tue 18:30 P1A

**Polarization-dependent ARPES investigation for organic molecules on Ag(110) and Cu(110)** — ●XIAOSHENG YANG<sup>1</sup>, DANIEL LÜFTNER<sup>2</sup>, GEORG KOLLER<sup>2</sup>, PETER PUSCHNIG<sup>2</sup>, MICHAEL RAMSEY<sup>2</sup>, MATTEO JUGOVAC<sup>3</sup>, GIOVANNI ZAMBORLINI<sup>3</sup>, VITALIY FEYER<sup>3</sup>, SERGUEI SOUBATCH<sup>1</sup>, and STEFAN TAUTZ<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGL-3), Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Institut für Physik, Karl-Franzens-Universität Graz, 8010 Graz, Austria — <sup>3</sup>Elettra-Sincrotrone Trieste, 34149 Basovizza, Trieste, Italy

The angle-resolved photoemission spectroscopy (ARPES) is often used to study electronic properties of molecule/metal interfaces. In particular, for planar  $\pi$ -conjugated molecules, utilizing a plane wave approximation for the photoelectron final states, it is possible to completely reconstruct the spatial distribution of the molecular orbitals [1,2]. However, recently it has been shown that the plane wave approximation fails to describe correctly the angular distribution of photoemission induced by the s-polarized light [3] and a better final states approx-

imation is needed to predict experimentally observed photoemission patterns. In this contribution, we revisit this issue and report on ARPES measurements of monolayers of several molecules - tetracene, pentacene, pentaphenyl and sexiphenyl - on Ag(110) and Cu(110) surfaces, performed using various polarizations of the incident light.

[1] P. Puschnig et al. *Science* 326, 702 (2009)

[2] S. Weiß et al. *Nature Comm.* 6, 8287 (2015)

[3] M. Dauth et al. *Phys. Rev. Lett.* 117, 183001 (2016)

O 46.20 Tue 18:30 P1A

**Ab-initio investigation of the interface  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>/Al** — ●LILIT AMIRKHANYAN and JENS KORTUS — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

Ceramic materials are used in industry to remove non-metallic inclusions from metallic melts like iron or aluminum. The filtration effect depends on interactions at the interface of the ceramic filter material. Interestingly, different ceramic materials show different filtration efficiency. Therefore, a detailed understanding of the processes at the interface are of interest.

We investigated the interface of the stable phase  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> with surface (0001). A model of the Al melt has been derived from bulk Al using the (111) plane. All calculations are based on density function theory as implemented in the Quantum Espresso code. In order to investigate the effect of oxygen or aluminum termination we carried out calculation on Al<sub>2</sub>O<sub>3</sub> with these two terminations using the Effective Screening Medium Method with open boundary conditions. As a result we find that both terminations will give positively charged surfaces.

Further, we created interface structures and obtained from these models an interface energy. The interface energy depends on the termination of  $\alpha$  - Al<sub>2</sub>O<sub>3</sub>. In particular, the oxygen terminated interface of  $\alpha$  - Al<sub>2</sub>O<sub>3</sub>/Al is more stable compared to the aluminum terminated case.

O 46.21 Tue 18:30 P1A

**The geometric and electronic properties of the tetracene/Ag(110) interface studied by density functional theory** — ●JANA FUCHSBERGER<sup>1</sup>, DANIEL LÜFTNER<sup>1</sup>, XIAOSHENG YANG<sup>2</sup>, GEORG KOLLER<sup>1</sup>, MICHAEL RAMSEY<sup>1</sup>, VITALIY FEYER<sup>3</sup>, SERGUEI SOUBATCH<sup>2</sup>, STEFAN TAUTZ<sup>2</sup>, and PETER PUSCHNIG<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Graz, Austria — <sup>2</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — <sup>3</sup>Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany

Recently, the puzzling question of tetracene monolayers on Ag(110) has been revisited by means of photoemission tomography experiments. Thereby the azimuthal orientation of the molecules has been studied and several molecular emissions have been identified. However, the origin of two distinct emissions separated by almost 1 eV that appear to have the photoemission distribution of the highest occupied molecular orbital (HOMO) could not be explained. In this contribution, we use density functional theory to shed light on this problem. First, we determine the optimal adsorption geometry for two molecular orientations, namely parallel and perpendicular to the close-packed Ag-rows. We further analyze their electronic structures in terms of work function modifications, charge rearrangements and projected density of states. Finally, we compare simulated photoemission momentum maps for the two structures with experimental data.

O 46.22 Tue 18:30 P1A

**DFT calculations of energy dependent XPS valance band spectra** — ●MAHDIYAR BAGHERI and PETER BLAHA — Institute of Materials Chemistry, Technical University Vienna, Vienna, Austria

In the past few years it became regularly possible to measure valance

band X-ray photoelectron spectra (XPS) using variable excitation energies. In order to explain the observed variations in intensity with respect to the excitation energy, we performed XPS calculations using the WIEN2k code. The new module computes the XPS spectra using a combination of partial density of states times excitation-energy-dependent atomic cross-sections, and considers as additional correction the fraction of the corresponding orbital contained inside the atomic spheres. The resulting XPS spectra are compared with experimental data for SiO<sub>2</sub>, PbO<sub>2</sub> and NiO at different excitation energies.

O 46.23 Tue 18:30 P1A

**Local effects of self-assembled monolayers on NiO thin films** — ●WENLAN LIU<sup>1,2</sup>, SHUANGYING MA<sup>1,2</sup>, SABINA HILLEBRANDT<sup>2</sup>, FLORIAN ULLRICH<sup>2</sup>, SEBASTIAN HIETZSCHOLD<sup>2</sup>, and ANDREAS KÖHN<sup>1,2</sup> — <sup>1</sup>Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart — <sup>2</sup>InnovationLab GmbH, Speyerer Straße 4, D-69115 Heidelberg

Due to the large band gap and the p-type character, NiO has been used as hole transmission and electron blocking layers in enhancing bulk heterojunction (BHJ) organic photovoltaic (OPV) cell performance. The performance of electronic devices can be further improved by applying self-assembled monolayer (SAM) on the NiO surface, such that one can easily tune the work function of the surface, and achieve other functions e.g. passivation and better wettability.[1]

As this work is closely cooperated with experiments based on solution-processed NiO thin films, we consider not only the idea NiO(111) surface, but also different variation of non-idea surfaces either with surface reconstruction or defect in buffer. Such local effects are taken care of by the periodic electrostatic embedded cluster model (PEECM).[2] The energetically stable conformations of the SAMs on NiO(111) surfaces have been examined. The corresponding properties have been calculated and compared carefully with the experimental results.

[1] S. A. DiBenedetto et al., *Adv. Mater.*, 21 (2009), 1407

[2] M. Sierka et al., *J. Chem. Phys.*, 120 (2009), 174710

O 46.24 Tue 18:30 P1A

**Self-assembled monolayers on NiO thin films: a first-principles study** — ●SHUANGYING MA<sup>1,2</sup>, WENLAN LIU<sup>1,2</sup>, SABINA HILLEBRANDT<sup>2</sup>, FLORIAN ULLRICH<sup>2</sup>, SEBASTIAN HIETZSCHOLD<sup>2</sup>, and ANDREAS KÖHN<sup>1,2</sup> — <sup>1</sup>Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart — <sup>2</sup>InnovationLab GmbH, Speyerer Straße 4, D-69115 Heidelberg

The study of the organic solar cells (OSC)[1]has received increasing attention due to its low cost and compatibility with the present well developed technologies[2]. NiO is good anode interlayer candidate owing to its wide band gap and p-type character[3]. By forming self assembled monolayers of certain organic molecules, e.g. 4-cyanophenyl phosphonic acid (CYNOPPA) on the NiO surface, can further modify the energy-level alignment between the semiconducting organic/inorganic interfaces, which is critical for efficient charge separation and significantly affects the open-circuit voltage as well[4].

In the present study, first-principles calculations are performed for different neat and SAMs modified hydroxylated and reconstructed NiO(111) surfaces. The related electronic and optoelectronic properties, e.g. band gaps, density of states, work functions, XPS and IR spectrums are compared with each other and with the experimental results. The corresponding dehydration mechanism between the CYNOPPA and NiO(111) hydroxylated surface is also studied with ab initio molecular dynamics.

[1] *Nat. Photon.*, 3 (2009), 649; [2] *Chem. Mater.*, 23 (2011) 2218;

[3] *Phys. Rev. B*, 75 (2007), 241203; [4] *Adv. Mater.*, 21 (2009), 1450