O 67: Poster: Electronic Structure of Surfaces

Time: Wednesday 18:00–20:00 Location: P2/EG

O 67.1 Wed 18:00 P2/EG

Fermi-level pinning at InP(001):H surfaces — •Rachele Sciotto, Isaac Azahel Ruiz Alvarado, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Stable InP(001):H surfaces are characterized by fully occupied and empty surface states close to the bulk valence and conduction band edges, respectively [1]. However, photoemission shows a surface Fermi level pinning at midgap energy [2]. In order to resolve that apparent discrepancy, we perform density-functional calculations. Ab initio thermodynamics is used to determine the density of surface defects as a function of temperature and hydrogen pressure. The influence of spin polarization and charging on the electronic properties of the surface defects is studied in detail. It is found that in particular P dangling bonds resulting from H desorption give rise partially filled midgap electronic states that are suitable to explain the experimental findings.

[1] WG Schmidt, et al. Phys. Rev. Lett. 90, 126101 (2003); PH Hahn, WG Schmidt, Surf. Rev. Lett. 10, 163 (2003).

[2] DC Moritz, et al. ACS Appl. Mater. Interfaces 14, 47255 (2022).

O 67.2 Wed 18:00 P2/EG

Dielectric anisotropy of heteroepitaxial GaP/AlP films grown on Si(001) from first-principles calculations — •Max Grossmann and Erich Runge — Technische Universität Ilmenau, Ilmenau, Deutschland

Low-defect III-V semiconductor films grown on Si(001) create new opportunities for cost-effective high-performance photovoltaic and optoelectronic devices. The recent work of Nandy et al. [1] shows a route how to drastically reduce the defect concentration of such structures through a thin GaP/AlP buffer layer. The growth of the latter is best monitored via reflection anisotropy spectroscopy (RAS). The theoretical characterization of RAS spectra is therefore vital for the monitoring of semiconductor growth processes as well as the understanding and improvement thereof. For these reasons we analyse the dielectric anisotropy for the case of a GaP/AlP/Si(001) heterostructure through first-principles calculations and compare them to the RAS measurements of Ref. [1]. [1] M. Nandy, A. Paszuk, M. Feifel, C. Koppka, P. Kleinschmidt, F. Dimroth, and T. Hannappel, A Route to Obtaining Low-Defect III/V Epilayers on Si(100) Utilizing MOCVD, Crystal Growth & Design 21, 5603-5613 (2021), 10.1021/acs.cgd.1c00410

O 67.3 Wed 18:00 P2/EG

Photoemission study of a Te Kagome adatom lattice on Pt(111) — •Nicolai Taufertshöfer[1,2], Begmuhammet Geldiyev[1,2], Maximilian Ünzelmann[1,2], Andreas Raabgrund[3], Tilman Kisslinger[3], Lutz Hammer[3], M. Alexander Schneider[3], Hendrik Bentmann[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, JMU Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg — [4]Center for Quantum Spintronics (QuSpin), NTNU Trondheim

Kagome lattices can host a variety of exotic phenomena such as flat bands, topological Dirac physics, or unconventional superconductivity [1]. In this contribution, we investigate the electronic structure of a Pt(111)-(3x3)-Te structure. This phase corresponds to a Kagome adlayer on a strongly reconstructed Pt(111) surface as determined by quantitative LEED-IV and STM. Utilizing angle-resolved photoemission spectroscopy, we find a Fermi surface with a rich structure stemming from a complex manifold of bulk and surface electronic states. Intending to unravel the influence of the Kagome lattice on the surface electronic band structure, we will carefully analyse and discuss our photoemission data. Particular attention will be on the nature of a band located in the close vicinity of the Fermi level at the center of the surface Brillouin zone.

[1] T. Neupert et al., *Nature Physics* **18**, 137-143 (2022)

O 67.4 Wed 18:00 P2/EG

Spin asymmetries in photoemission from $PtTe_2$. — •Muthu Prasath Thirugnanasambandam Masilamani[1], Jakub Schusser[1], Mohammed Qahosh[2], Gustav Bihlmayer[3], Lukasz Plucinski[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, Jülich, Germany

In our recent work [1], we addressed the occurrence of spin-resolved photoemission signal asymmetries in the Weyl type-II semimetal candidate WTe_2. Here, we aim to understand the asymmetric spin texture of electrons photoemitted from surface and bulk states and its relation to the initial state of type-II Dirac semimetal $PtTe_2$ with photon energy of $h\nu = 21.22$ eV at room temperature and at 50K. Our spin- and angle-resolved photoemission data were augmented by the one-step model of the photoemission within the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) Green's function method of the Munich band structure software package. In order to extract information about the different contributions to the resulting spectral weight and spin polarization, the matrix-element used in our one-step model of photoemission calculations includes all experimental parameters such as photon energy, light polarization and geometry configurations.

[1] T. Heider et al., arXiv:2210.10870 (2022).

O 67.5 Wed 18:00 P2/EG

Quasiparticle lifetime and formation of electronic states at Tellurium–metal interfaces — •Begmuhammet Geldiyev[1,3], Maximilian Ünzelmann[1,3], Philipp Eck[2,3], Domenico Di Sante[2,3], Giorgio Sangiovanni[2,3], Thomas Fauster[4], Hendrik Bentmann[1,3], and Friedrich Reinert[1,3] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Theoretische Physik 1, Universität Würzburg — [3]Würzburg-Dresden Cluster of Excellence ct.qmat — [4]Lst. f. Festkörperphysik, Universität Erlangen-Nürnberg

Properties of interfaces between a device material and metallic contacts can decisively influence the resulting device performance. In particular, the formation of electronic interface states (IS) with short lifetimes could speed up the charge carrier injection [1]. In this contribution, we will discuss the formation of IS at Te – noble metal interfaces, i.e., particularly in a suitable model system AgTe / Ag(111) [2]. Utilizing one- and two-photon photoemission, we find that hybridizations between Te-p_z orbitals with substrate bulk and surface states determine the interface electronic structure. Whilst the AgTe valence band states are located almost completely within the AgTe layer, the wave function of the unoccupied state γ, lying 530 meV above E_F within the projected bulk band gap, has a sizable overlap with the substrate states. Evidence is provided by a rather short lifetime $\tau = 31 \pm 3$ fs of γ as well as by light-polarization-dependent measurements revealing the orbital character of the occupied and unoccupied states.

[1] C. H. Schwalb et al., Phys. Rev. Lett. 101, 146801 (2008)

[2] M. Ünzelmann et al., Phys. Rev. Lett. 124, 176401 (2020)

O 67.6 Wed 18:00 P2/EG

Accelerating plane-wave-based *ab initio* molecular dynamics by optimization of Fast-Fourier transforms for modern HPC architectures — •Christian Ritterhoff, Tobias Klöffel, Sagarmoy Mandal, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

The most important advantage of plane-wave basis sets is that wave functions can be transformed efficiently from reciprocal to real space and back by using the Fast-Fourier transform (FFT) algorithm. This allows to evaluate the kinetic and potential energy in reciprocal and real space, respectively, where both operators are diagonal. This reduces the computational cost for applying the Hamilton operator from N^2 to $N \log N$. However, the scalability of current FFT libraries is rather limited on today's HPC systems, which offer large numbers of compute nodes, each of them with many cores. Here we present our optimization of the FFTX library of the Quantum Espresso software package. Data distribution and communication patterns have been revised to make optimal use of combined MPI and OpenMP parallelization. Scalability is further increased by combining FFTs into batches and by introducing overlapping computation and communication. We implemented the revised FFTX library in our optimized version of the CPMD code [1], and we demonstrate the achieved acceleration by a

series of benchmark simulations.

[1] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745

O 67.7 Wed 18:00 P2/EG

Comparison of machine learning strategies in the high-throughput exploration of $AB\mathbf{O}_2$ delafossites — •Armin Sahinovic, Benjamin Geisler, and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen

The advent of machine learning introduced new techniques to considerably expedite materials discovery. This raises a fundamental question about how they balance interpretability versus accuracy. We address this aspect by comparing ensemble-based active learning (AL) of neural networks (NN) [1] and the sure independence screening and sparsifying operator (SISSO) [2] for the prediction of formation energies and lattice parameters in $AB\mathrm{O}_2$ delafossite oxides. To this end, we generate a consistent dataset from first principles. Element embedding is found to be superior to scalar input strategies, e.g., atomic properties. In conjunction with AL, the NNs reach DFT accuracy, allowing for a significant acceleration of high-throughput materials screening. In contrast, the precision of the physically interpretable SISSO descriptors is limited by the high data complexity. We combine $AB\mathrm{O}_2$ infinite-layer, $AB\mathrm{O}_3$ perovskite [1] and the delafossite data to extend the unsupervised AL into the structural space, thereby enhancing the sample efficiency in the spirit of transfer learning. Finally, we compile a phase diagram that compares the relative stability of the three distinct oxide materials classes.

[1] A. Sahinovic and B. Geisler, Phys. Rev. Research 3, L042022 (2021); J. Phys.: Condens. Matter 34, 214003 (2022)
[2] R. Ouyang *et al.*, Phys. Rev. Materials 2, 083802 (2018)

O 67.8 Wed 18:00 P2/EG

Spin-polarized very-low-energy electron diffraction from spin-orbit- and/or exchange-influenced targets — •Christoph Angrick[1], Christian Thiede[1], Andre Reimann[1], Annika Henriksen[1], Nicole Mutzke[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2], and Markus Donath[1] — [1]University of Münster, Germany — [2]BTU Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

Exchange (XC) or spin-orbit (SOC) interaction cause electron scattering from surfaces to be spin dependent. The resulting spin filtering of the scattered electron beam can be used in spin-polarization analyzers. These analyzers are implemented in, for instance, photoemission setups to obtain spin resolution. Therefore, for promising targets, electron reflectivity and resulting spin asymmetry of very-low-energy electrons are measured for a wide range of incident electron energies and angles. By this, the investigated target is put to a test regarding the usability as a scattering target in a spin-polarization analyzer.

Here, several results of SOC- as well as XC-influenced targets are presented. The results of the SOC-influenced targets Au(111), single-layer MoS_2/Au(111) and W(110) [1] are compared with the results of the XC-influenced target Fe(001)-p(1x1)O [2]. Additionally, the influence of SOC interaction in the case of the XC-influenced target is investigated. The spin asymmetry caused by SOC is found to be one order of magnitude smaller than the spin asymmetry caused by XC.

[1] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).
[2] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).

O 67.9 Wed 18:00 P2/EG

Exploring electronic structural properties of Copper(Cu) via Auger Photoelectron Coincidence Spectroscopy — •Swarnshikha Sinha[1,2], Danilo Kühn[1], and Alexander Föhlisch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [2]Universität Potsdam, Institut für Physik und Astronomie

The electronic structure of the 3d transition metals are immensely influenced by many electron effects. Photoemission spectroscopy (PES) and Auger electron spectroscopy (AES) can help to learn about screening processes in core excited states and electron correlations in two-hole final states, respectively.

However, in Cu 3p photoemission and MVV Auger decay, the final state holes are located in the same main shell as the initial vacancy, leading to strong lifetime broadening in the spectra. APECS, can help in reducing lifetime broadening and revealing overlapping spectral features. [1] A comparative study of three different copper surfaces (111,110 and 100) was conducted using APECS, at the COESCA station, UE52 PGM beamline at BESSYII [2].Our results confirm a strong energy sharing between the Photo and Auger electrons [3]and substantial differences in the screening of the final states, leading to different asymmetry of the atomic multiplet peaks in the two-hole spectra of the three Cu surfaces.

[1] H.W. Haak, et al., Phys. Rev. Lett. 41, 1825 (1978) [2] T. Leitner, et al., J. El. Spec. 250, 147075 (2021) [3] E. Jensen, et al., Phys. Rev. Lett. 62, 71 (1989)

O 67.10 Wed 18:00 P2/EG

Improved convergence of the density response function by an incomplete-basis correction — •Jörn Stöhler[1,2], Markus Betzinger[1], Stefan Blügel[1], and Christoph Friedrich[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]RWTH Aachen University, Germany

The polarizability (or density response function) is a central quantity in many electronic structure methods, e.g., the *GW* approach, the random-phase-approximation (RPA) total-energy method, the optimized effective potential method, the Bethe-Salpeter approach, Coulomb-hole screened-exchange (COHSEX). In time-dependent perturbation theory, the polarizability can be expressed as a sum over unoccupied states. However, the resulting sum-over-states expression converges very slowly with respect to the number of bands or the basis-set size, in particular, in systems containing localized *d*- and *f*-states. Here, we discuss a method, called incomplete-basis-set correction [1,2], which augments the sum-over-states expression with a numerical solution of the radial Sternheimer equation in the atomic (muffin-tin) spheres. The method is implemented in the `Spex` code within the FLAPW approach. The resulting polarizability shows a considerably improved convergence behavior with respect to the basis set and the number of unoccupied states.

[1] M. Betzinger, C. Friedrich, A. Görling, S. Blügel, Phys. Rev. B **85**, 245124 (2012), *ibid.* Phys. Rev. B **92**, 245101 (2015).
[2] M. Betzinger, C. Friedrich, S. Blügel, PRB **88**, 075130 (2013).