TT 55: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Wednesday 15:00–18:30 Location: H24

Topical Talk TT 55.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — Tomáš Rauch[1], Steven Achilles[1], •Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of "original" TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ± 1; their projections onto the surface Brillouin zone are connected by a Fermi arc, i. e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained $HgTe_{1-x}S_x$ alloys [1], with surprising results. (*i*) In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x. (*ii*) On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the "topological playground" for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk TT 55.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — •Binghai Yan — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monopnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B 92, 115428 (2015). [2] L. X. Yang, et al. Nature Physics 11, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics 11, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

TT 55.3 Wed 16:00 H24

Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe_2 — •Lukas Muechler[1], Aris Alexandradinata[2], Titus Neupert[3], and Roberto Car[1] — [1]Dept. of Chemistry, Princeton University — [2]Dept. of Physics, Yale University — [3]Princeton Center for Theoretical Science, Princeton University

WTe_2 is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm^2/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe_2 based on Wannier functions from *ab-inito* calculations and extend our findings to the iso-structural compounds $MoTe_2$ and ZrI_2.

TT 55.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully ab initio calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

[1] L. X. Yang, Z. K. Liu, Y. Sun, et. al. Nat.Phys.11,728, (2015).

[2] Z. K. Liu, L. X. Yang, Y. Sun, et.al Nat. Mater., doi:10.1038/nmat4457,(2015).

[3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, 92, 115428, (2015).

TT 55.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — •L Nicolaï[1,2,3], K Hricovini[2,3], J-M Mariot[4], M C Richter[2,3], O Heckmann[2,3], U Djukic[2], T Balasubramanian[5], M Leandersson[5], J Sadowski[5], J Denlinger[6], I Vobornik[7], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LMU, Munich — [2]LPMS, UCP, Cergy, France — [3]DSM-IRAMIS, Spec, Cea-Saclay, France — [4]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [5]MAX-lab, Lund Univ., Sweden — [6]ALS, Berkeley, USA — [7]EST, Trieste, Italy — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states.[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

TT 55.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from *GW* calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 with thicknesses from one to six quintuple layers employing the *GW* method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing $\mathcal{H}^{\mathrm{QP}}$. The origin of the respective

off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in *GW* differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

TT 55.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — •Stefan Kurth[1,2] and Gianluca Stefanucci[3,4] — [1]Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — [4]INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

TT 55.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — •Giuseppe Foti and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)
[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

TT 55.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — •Zhi Wang[1], Shu-Shen Li[2], and Lin-Wang Wang[3] — [1]Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [3]Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge seperations in photovoltaic systems.

TT 55.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — •Ryan Requist and Eberhard K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions "smear out" the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys. Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

TT 55.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

TT 55.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — •Thorsten Deilmann, Matthias Drüppel, and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.
We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used *GW* method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.
We investigate trion states in a semiconducting $(8, 0)$ carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by $\sim 135\,\text{meV}$ compared to the excitons.