**HL 51: Topological Insulators II (jointly with MA, DS, O, TT)**

**Time:** Wednesday 9:30–13:00  
**Location:** EB 301

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**HL 51.1 Wed 9:30 EB 301**

Probing the topological states of Sb$_2$Te$_3$ by spin polarized photoemission spectroscopy — Christian Pauly$^1$, GUSTAV BILHMAYER$^2$, MARCUS LIEBMANN$^3$, DINESH SUBRAMANIAN$^4$, MARTIN GROß$^1$, ALEXANDER GEORGII$^1$, MARKUS SCHÖLL$^1$, JAIME SANCHEZ BARRIGA$^4$, STEFAN BLÖGEL$^5$, OLIVER RADER$^5$, and MARKUS MORGENSTERN$^1$  

**First-principle study**

Topologically-related properties in presence of disorder.  

Based on first-principle calculations involving the Coherent Potential Approximation (CPA), we inspect the disorder-affected transport properties of the random alloys between topologically non-trivial and trivial materials. The subsequent analysis encounters few interesting aspects: the way how to increase the Hall angle by using random disorder and an indication for the topological Anderson insulator. In addition CPA provides an alternative recipe to validate the non-trivial order and an indication for the topological Anderson insulator.

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**HL 51.2 Wed 9:45 EB 301**

Electronic properties and magnetic anisotropy of individual Co adatoms adsorbed on topological insulator surfaces — T. ELSER$^3$, M. SEPEHR$^1$, M. WÖRLE$^1$, M. DÖRLE$^3$, M. GYAMFI$^1$, G. BILHMAYER$^2$, I. MIOTKOWSKI$^4$, A. KOZŁOWSKI$^2$, and R. WIENENDANGER$^1$  

**HL 51.3 Wed 10:00 EB 301**

Theoretical study on the reactive chemical doping of the Bi$_2$Se$_3$ surface — YANOS KISS$^{1,2}$, STANISLAV CHADOV$^{1,2}$, and CLAUDIA FELSER$^{1,2}$  

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**HL 51.5 Wed 10:30 EB 301**

Heusler topological insulators: Electronic structure and transport properties — C. SHEKHAR$^1$, S. OUARDI$^2$, G. H. FECHER$^{1,2}$, A. K. NAYAK$^1$, A. GLOSKOVSKI$^2$, E. IKENAGA$^3$, S. UEDA$^4$, K. KOSAYASHI$^4$, and C. FELSER$^{1,2}$  

**HL 51.6 Wed 10:45 EB 301**

Topological phase transitions in Bi(111) bilayer by breaking time-reversal symmetry — HONGBIN ZHANG, FRANK FREIMUTH, GUSTAV BILHMAYER, STEFAN BLÜGEL, Daniel DÖRLE, M. GYAMFI, and MAURICE MOKROUSOV  

**HL 51.7 Wed 11:00 EB 301**
Predicting surface states from the bulk embedding self-energy — Daniel Wortmann, Gustav Blügel, and Stefan Blügel — Institute for Advanced Simulation & Peter Grünberg Institut, Forschungszentrum Jülich und JARA, 52425 Jülich, Germany

The protected states localized at surfaces and interfaces of topological insulators are a consequence of the electronic structure of the bulk. Their peculiar features like the typical spin-structure makes them an interesting field of basic research with possible applications in spintronics.

We demonstrate how these states can be efficiently simulated by means of the embedding self-energy as obtained in the Green function embedding technique[1]. The embedding self-energy, which can be understood as a generalized logarithmic derivative, is a property of the bulk crystal only and contains all information required to analyze the consequences of the bulk topology on the surface bandstructure. Using the FLAPW implementation of the embedding method as provided in the FLEUR-code[2], we show how the surface states of prototypical topological insulators like Bi2Se3 can be studied efficiently with an easy and direct access to effects for example due to electric fields applied to the surface.


15 min. break

HL 51.8 Wed 11:30 EB 301

Influence of magnetic impurities on doping and scattering properties of topological surface states: Fe on Bi2Te3 (X=Te, Se) — Markus R. Scholz1, J. Sánchez-Barriga1, D. Marchenko1, A. Varykhalov1, E. Rienks2, A. Volykovich2, L. V. Yashina2, and O. Rader3

We study the effect of Fe impurities deposited on the surface of the topological insulators Bi2Se3 and Bi2Te3 by means of photoelectron spectroscopy. The topological surface state reveals surface electron doping when the Fe is deposited at room temperature and hole doping when deposited at low temperature (∼10 K). We show that in both cases the topological surface state remains intact and gapless.

We analyze the line broadening for pure Bi2Te3 (X=Se, Te) and after deposition of Fe. We observe that the constant broadening in the bulk band gap range increases by a factor of 2 upon deposition of Fe. Because we deposit the Fe without electron doping, this result is not due to a gain in warping as was recently suggested. We discuss the results based on different types of scattering mechanisms.

HL 51.9 Wed 11:45 EB 301


— Helmholtz-Zentrum Berlin — Moscow State University

We have recently reported a strong circular dichroism effect in angle-resolved photoemission of the spin polarized topological surface state of Bi2Te3 [1]. The effect has been observed recently also for Bi2Se3 and the origin is controversial [2-4]. An initial-state model has been employed to determine the spin orientation directly [3]. We present a series of photoemission measurements and density functional calculations coupled to one-step photoemission theory. Both experiment and theory reveal that the dichroism effect changes sign as a function of photon energy which excludes the initial-state model.


HL 51.10 Wed 12:00 EB 301

Prediction of topological insulators in TIBi2Se2 family of chalcogenides — Binhai Yan — BCCMS, University of Bremen, Bremen

In this work, we predicted several new topological insulator materials in thallium (Tl) based ternary chalcogenides from first-principles calculations, including TIBi2Q and TISb2Q (Q=Te, Se and S). TIBi2Se and TISb2Se are found to be strong TIs with a large energy gap (∼0.2 eV), while TIBi2Te is a topological semimetal. A simple Dirac-type dispersion of topological surface states is observed, similar to the Bi2Se3c type of materials. On the other hand, TIBi2S2, TISb2Te and TISb2S2 are small gap insulators near the topological trivial-nontrivial transition boundary. Particularly TIBi2Te2 can be a good candidate in the seeking of Majorana fermions for its co-existing superconductivity property. The topological feature of TIBi2Se and TIBi2Te has already been confirmed by recent experiments. References: 1. B. H. Yan, C. X. Liu, H. J. Zhang, C. Y. Yan, X. L. Qi, Th. Frauenheim and S. C. Zhang, Europhys. Lett. 90, 37002 (2010). 2. Y. L. Chen, Z. K. Liu, J. G. Analytis, J.-H. Chu, H. J. Zhang, B. H. Yan, S.-K. Mo, R. G. Moore, D. H. Lu, I. R. Fisher, S. C. Zhang, Z. Hussain, and Z.-X. Shen. Phys. Rev. Lett. 105, 266401 (2011).

HL 51.11 Wed 12:15 EB 301

A recipe for new Topological Insulators based on bonds, bands, symmetry and heavy atoms — Øl. Mückler, B. Yan1, S. Chadov1, A. Volykhov, C. Felser

— Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg University Mainz — Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045, USA — Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

In this work we will present a recipe for finding new Topological Insulators (TI) based on bonds, bands, symmetry and heavy atoms. A big issue concerning the compounds known up to now is the control of the bulk carrier density to produce truly insulating samples in the bulk. Using concepts from chemistry and supported by density-functional calculations, we want to motivate an extended search for new compounds with tunable bulk properties.

HL 51.12 Wed 12:30 EB 301

Graphene nanoribbons with Au induced spin-orbit effects: a DFT study — Gustav Blügel and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich und JARA, 52425 Jülich, Germany

Historically, the prediction of a topological protection of the edge state of a zig-zag graphene nanoribbon (ZGNR) was at the beginning of the field of topological insulators. Unfortunately, a realization of this system is prevented by (i) the extremely small spin-orbit coupling (SOC) in graphene and (ii) the tendency towards formation of antiferromagnetically coupled edge states in ZGNRs.

New experimental and theoretical results show that SOC effects can be enhanced by substrates and/or adatoms with a large atomic number, so that up to 100 meV spin-splitting can be realized in the graphene. Additionally, hybridization with the substrate changes also the localization of the edge state and its tendency towards antiferromagnetic ordering. Density functional theory calculations of Au supported graphene (with and without adatoms) and ZGNRs will illustrate these effects and point the way towards a realization of a ZNGR with a topologically protected edge state.

HL 51.13 Wed 12:45 EB 301

Collision dominated scattering in 3D topological insulators — Peter Lemmens, Vladimir Gnezdilov, Dirk Wüster, Yuriy Pashkevich, Ekaterina Pomjakushina, Kazimir Conder, and Helmuth Berger — IPK, TU-BS, Braunschweig, Germany — ILTPE NAS, Ukraine — DonFTI, Donetsk, Ukraine — PSI, Villigen, Switzerland — EPFL, Lausanne, Switzerland

Despite topological protection in 3D topological insulators there exist scattering processes induced by a resonant excitation from a bulk valence band to Dirac states. This so-called scattering is a Lorentzian lineshape and spin-helical symmetry with a scattering rate of 40 cm−1. A comparison of different compounds (Bi2Se3, Bi2Te3), substitution experiments as well as first results on BiTeI with giant Rashba spin splitting are presented. Work supported by DFG and NTH.