

HL 67: Topological insulators I (MA with HL/TT)

Time: Thursday 9:30–12:00

Location: EB 202

HL 67.1 Thu 9:30 EB 202

DETECTION OF SURFACE SPIN CURRENT IN 3-DIMENSIONAL TOPOLOGICAL INSULATOR, BiSbTeSe— ●MASASHI SHIRAIISHI¹, YUICHIRO ANDO¹, TAKAHIRO HAMASAKI¹, KOHJI SEGAWA², SATOSHI SASAKI², FENG YANG², MARIO NOVAK², and YOICHI ANDO² — ¹Kyoto Univ., Japan — ²ISIR, Osaka Univ., Japan

Topological insulators (TIs) attract tremendous attention in recent years, since topologically-protected edge current is a persistent pure spin current. The first detection of the edge current was achieved by using 2-dimensional TI, HgTe quantum well [1], and the next challenge is to detect the edge current in 3-dimensional TIs, because a number of spin channel can be dramatically increased. Whereas Li et al. claimed that they successfully detected the surface spin current in Bi₂Se₃ by using an electrical spin accumulation method [2], the polarity of the spin signals is not accordance with the direction of magnetization of a detector ferromagnet. Thus, there is still open for discussion how to detect the edge spin current. Here, we present the detection of the edge spin current of BiSbTeSe, which is a bulk insulative TI [3]. The spin signal due to the spin accumulation was detected electrically, and was observed up to 150 K [4].

[1] M. Koenig et al., *Science* 318, 766 (2007). [2] C. Li et al., *Nature Nanotech.* 9, 218 (2014). [3] T. Arakane, Yo. Ando et al., *Nature Commun.* 3, 636 (2011). [4] Yu. Ando, M. Shiraishi et al., *Nano Lett.*, in press.

HL 67.2 Thu 9:45 EB 202

First-principles calculation of quasiparticle spin interference and scattering processes on 3D topological insulators

— ●PHILIPP RÜSSMANN, PHIVOS MAVROPOULOS, NGUYEN H. LONG, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present density-functional calculations of the quasiparticle interference (QPI) due to scattering of electrons off magnetic and non-magnetic impurities at the surface of the strong topological insulator Bi₂Te₃. The focus of our work is the calculation and analysis of possible spin-dependent scattering processes and their relation to the QPI pattern observed in experiment. The presence of an impurity magnetic moment leads to broken time-reversal symmetry and the protection against back-scattering is lifted. Therefore, we investigate magnetic transition-metal adatoms as well as non-magnetic Bi and Te adatoms on Bi₂Te₃. Finally, we compare the QPI pattern and scattering processes at different energies around the Fermi energy and discuss the importance of the hexagonal warping of the constant energy contours.

The electronic structure calculations are carried out with our KKR-Green function method for scattering properties at defects [1]. We acknowledge financial support from the DFG (SPP-1666), from the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre at the RWTH Aachen University.

[1] N. H. Long, P. Mavropoulos, B. Zimmermann, D. S. G. Bauer, S. Blügel, and Y. Mokrousov, *Phys. Rev. B* 90, 064406 (2014).

HL 67.3 Thu 10:00 EB 202

Momentum resolved spin dynamics of bulk and surface excited states in the topological insulator Bi₂Se₃— C CACHO¹, A CREPALDI², M BATTIATO³, J BRAUN⁵, H EBERT⁵, K HRICOVINI⁴, ●JAN MINAR^{5,6}, and F PARMIGIANI² — ¹Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell, United Kingdom — ²Elettra - Sincrotrone Trieste, Italy — ³Institute of Solid State Physics, Vienna University of Technology — ⁴Universite de Cergy-Pontoise, France — ⁵LMU München, Germany — ⁶University of West Bohemia, Plzen, Czech Rep.

The prospective of optically inducing a spin polarized current for spintronic devices has generated a vast interest in the out-of-equilibrium electronic and spin structure of topological insulators (TIs). In this presentation we prove that only by measuring the spin intensity signal over several order of magnitude in spin, time and angle resolved photoemission spectroscopy (STAR-PES) experiments is it possible to comprehensively describe the optically excited electronic states in TIs materials. The experiments performed on Bi₂Se₃ reveal the existence of a Surface-Resonance-State in the 2nd bulk band gap interpreted

on the basis of fully relativistic ab-initio spin resolved photoemission calculations. Remarkably, the spin dependent relaxation of the hot carriers is well reproduced by a spin dynamics model considering two non-interacting electronic systems, derived from the excited surface and bulk states, with different electronic temperatures. For more details see: Cacho et al.,

<http://arxiv.org/abs/1409.5018>

HL 67.4 Thu 10:15 EB 202

Spin structure of the Dirac state of the topological insulator Bi₂Te₃(0001)— ●CHRISTOPH SEIBEL¹, HENRIETTE MAASS¹, HENDRIK BENTMANN¹, JÜRGEN BRAUN², JAN MINÁR², TAICHI OKUDA³, and FRIEDRICH REINERT¹ — ¹Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — ²Department Chemie, Physikalische Chemie, Universität München, Butenandtstrasse 5-13, D-81337 München — ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Three-dimensional topological insulators feature non-trivial surface states in the fundamental band gap of the bulk. In particular, the spin texture of these topological surface states (TSS) attracts attention in the context of possible applications in spintronics. We have performed angle- and spin-resolved photoemission measurements to analyze the three-dimensional spin texture of the TSS of the topological insulator Bi₂Te₃. The measured photoelectron spin-polarization is found to significantly deviate from the anticipated ground-state spin texture of the TSS, as derived e.g. on the basis of first-principles calculations. Possible origins of our observations are discussed in terms of the influence of spin-orbit coupling on the photoemission process. We compare our experimental data to the results of fully relativistic one-step photoemission calculations.

HL 67.5 Thu 10:30 EB 202

Atomic relaxations in Bi₂Se₃(0001)— SUMALAY ROY¹, ●HOLGER L. MEYERHEIM¹, KATAYOON MOHSENI¹, ARTHUR ERNST¹, MIKHAIL OTROKOV^{2,3}, MAIA G. VERGNIORY^{1,2}, GREGOR MUSSLER⁴, CHRISTIAN TUSCHE¹, EVGUENI CHULKOV^{2,3}, and JÜRGEN KIRSCHNER^{1,5} — ¹MPI f. Mikrostrukturphysik, D-06120 Halle, Germany — ²DIPC, San Sebastian, Spain — ³Tomsk St. Univ., Russia — ⁴FZ Jülich, Germany — ⁵MLU Halle-Wittenberg, Germany

Surface x-ray diffraction analysis of the Bi₂Se₃(0001) surface reveals an expansion of the top Se-Bi interlayer spacing in the range between 2 and 17% relative to the bulk. It is directly related to the concentration of surface contaminants like carbon and is observed in both, single crystals and MBE grown ultrathin films. Deeper layers and the first van der Waals gap remain unrelaxed. Ab-initio calculations which are in agreement with angular resolved photoemission experiments reveal that carbon acts as an n-dopant, while the top layer expansion induces a shift of the Dirac point towards the bulk conduction band of Bi₂Se₃ [1,2].

[1] S. Roy, H.L. Meyerheim, A. Ernst et al., *PRL* 113, 116802 (2014);

[2] S. Roy, H.L. Meyerheim, K. Mohseni et al., *PRB* 90, 155456 (2014)

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HL 67.6 Thu 10:45 EB 202

Spin resolved momentum microscopy of the topological insulator Bi₂Se₃— ●CHRISTIAN TUSCHE¹, MARTIN ELLGUTH¹, SHIGEMASA SUGA^{1,2}, HOLGER L. MEYERHEIM¹, and JÜRGEN KIRSCHNER^{1,3} — ¹Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — ²Institute of Scientific and Industrial Research, Osaka, Japan — ³Institut für Physik, Martin-Luther-Universität, Halle, Germany

Topological insulators are a new class of materials that attracted wide interest by their electronic structure with unusual relations of electron spin and momentum, leading to highly spin polarized “Dirac-cone” surface states. Recently, comprehensive experimental access to such band structures became feasible by spin resolved momentum microscopy. This novel concept combines high resolution imaging of photoelectrons in two-dimensional (k_x, k_y) sections with a highly efficient imaging spin filter. Electron reflection at a Au/Ir(100) mirror allows us to measure 5000 spin-resolved points in the surface Brillouin zone, simultaneously.

We show that the band-structure of Bi₂Se₃ is characterized by highly

spin polarized states within the complete Brillouin zone, beyond the “Dirac cone” surface state. For the latter we find that the spin polarization of photoelectrons can reach up to 90%, the highest value reported so far. A direct conclusion on the ground state polarization in these systems is complicated by the peculiar interplay between spin- and light-polarization in the photoemission, as directly observed in spin-resolved (k_x, k_y) images.

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HL 67.7 Thu 11:00 EB 202

The magnetism of Ni adatoms adsorbed on the TI $\text{Bi}_2\text{Te}_2\text{Se}$ — JAN HONOLKA¹, MARTIN VONDRÁČEK¹, •LASSE CORNILS², MALTE SCHÜLER³, MARKUS DUNST⁴, JONAS WARMUTH², LIHUI ZHOU², ANAND KAMLAPURE², ALEXANDER AKO KHAJETOORIANS^{2,5}, MATTEO MICHIARDI⁶, LUCAS BARRETO⁶, PHILIP HOFMANN⁶, JIAN-LI MI⁶, MARTIN BREMHOLM⁶, BO B. IVERSEN⁶, CINTHIA PIAMONTEZE⁷, HUBERT EBERT⁴, JAN MINAR^{4,8}, TIM WEHLING³, ROLAND WIESENDANGER², and JENS WIEBE² — ¹Inst. of Physics ASCR, Prague, Czech Republic — ²INF, University of Hamburg, Germany — ³Inst. of Theo. Physics, University of Bremen, Germany — ⁴LMU München, Germany — ⁵IMM, Radboud University Nijmegen, The Netherlands — ⁶iNano, Aarhus University, Denmark — ⁷PSI, Switzerland — ⁸New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

The predicted gap opening in the surface state of topological insulators (TIs) induced by surface magnetic doping, and the associated novel electron phases, have recently caught strong interest of the scientific community. However, the experimental evidence of an induced gap opening is still controversial [1] and calls for a detailed investigation of the magnetism of different adatoms. Here, we show by a combined XMCD, ARPES and STS study, that Ni adatoms on the TI $\text{Bi}_2\text{Te}_2\text{Se}$ reveal a surprising behaviour: While there is no detectable XMCD signal at the Ni $L_{2,3}$ -edges, the XAS spectrum unveils a considerable resonant absorption of the d-shell. The results are analyzed by *ab-initio* calculations. [1] J. Honolka *et al.*, PRL **108**, 256811 (2012).

HL 67.8 Thu 11:15 EB 202

Fe-induced stress on Bi_2Se_3 (0001) — •KENIA NOVAKOSKI FISCHER, SAFIA OUAZI, DIRK SANDER, and JÜRGEN KIRSCHNER — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

The topological insulator Bi_2Se_3 has attracted intense research activity since its discovery 5 years ago [1]. Here we present the first experimental study of the stress change induced by sub-monolayer deposition of Fe on Bi_2Se_3 . Deposition of 0.2 ML Fe at 300 K induces a stress change of -2.3 N/m. On the contrary, deposition of Fe at 150 K leads to negligible stress change of less than -0.2 N/m. The growth of Fe at 473 K induces a stress of -3.4 N/m. LEED reveals that the hexagonal diffraction pattern of the substrate gets blurred for deposition at 150 K, whereas deposition at higher temperature induces faint diffraction spots indicative of precursor of possible FeSe formation. We discuss these results in view of a recent STM study [2], where the authors suggest thermally activated sub-surface doping of Bi_2Se_3 by Fe.

[1] H. Zhang, C.X. Liu, X.L. Qi, X. Dai, Z. Fang, and S. C. Zhang, Nat. Phys. **5** (2009) 438; W. Zhang, R. Yu, H.J. Zhang, X. Dai, and Z. Fang, New Journal of Physics **12** (2010) 065013. [2] T. Schlenk, M. Bianchi, M. Koleini, A. Eich, O. Pietzsch, T. O. Wehling, T. Frauen-

heim, A. Balatsky, J.-L. Mi, B. B. Iversen, J. Wiebe, A. A. Khajetoorians, Ph. Hofmann, and R. Wiesendanger, Phys. Rev. Lett. **110** (2013) 126804

HL 67.9 Thu 11:30 EB 202

Atomic structure and magnetism of Fe on Bi_2Se_3 — •ANDREY POLYAKOV¹, HOLGER L. MEYERHEIM¹, E. DARYL CROZIER², ROBERT A. GORDON³, MAIA G. VERGNIORY⁴, ARTHUR ERNST¹, EVGUENI V. CHULKOV⁴, and JÜRGEN KIRSCHNER^{1,5} — ¹MPI f. Mikrostrukturphysik, D-06120 Halle, Germany — ²SFU, Burnaby, V5A 1S6 BC, Canada — ³CLS at APS Sector 20, Argonne, IL, USA — ⁴DIPC, San Sebastian, Spain — ⁵MLU Halle-Wittenberg, Germany

We have carried out extended x-ray absorption fine structure (EXAFS) and surface x-ray diffraction (SXRD) experiments in combination with *ab-initio* calculations to investigate the geometric and magnetic properties of iron deposited on the (0001) surface of the topological insulator Bi_2Se_3 in the coverage range between about 0.2 and 1.5 monolayers (ML). For iron deposited at $T=170$ K in the low coverage limit no polarization dependence of the EXAFS amplitude (electric field vector parallel vs. perpendicular to the surface of the bulk crystal) could be observed. In combination with the nearest neighbor distance of 2.42 Å this suggests that Fe atoms substitute bismuth atoms involving a local relaxation of the neighboring selenium atoms. *Ab-initio* calculations support this structural model and predict antiferromagnetic ordering of iron [1]. SXR data collected at 1.5 ML indicate that iron atoms also occupy threefold hollow surface sites. Mild annealing leads to the formation of a bulk FeSe like structure. [1] M. G. Vergniory *et al.* PRB **89**, 165202 (2014); This work is supported by SPP 1666 (Topological Insulators). Work at APS sector 20 is supported by the CLS and by US DOE under Contract No. DE-AC02-06CH11357

HL 67.10 Thu 11:45 EB 202

Signatures of Dirac fermion-mediated magnetic order

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The spin-momentum locking of topological states offers an ideal platform to explore novel magneto-electric effects. These intimately depend on the ability to manipulate the spin texture in a controlled way. Although numerous studies aimed to shed light on the role played by magnetic perturbations, contradictory results have been obtained and a clear picture is still missing. The interaction of surface magnetic moments with topological states has predominantly been performed by using spatial averaging techniques such as angle-resolved photoemission spectroscopy and x-ray magnetic circular dichroism. Here, we combine low-temperature scanning tunneling microscopy with single-adatom deposition to directly map the evolution of the electronic properties of topological states under the influence of different magnetic perturbations. By analyzing energy-resolved quasi-particle interference maps, we reveal signatures of Dirac fermion-mediated surface magnetic order for extremely dilute adatom concentrations. By using different magnetic elements and coverages, we find that this striking observation crucially depends on two parameters: single adatoms magnetic anisotropy direction and energy-level alignment [1].

[1] P. Sessi *et al.*, Nature Comm. **5**, 5349 (2014).