O 21: [MA] Joint Session "Topological Insulators I" (jointly with DS, HL, O, TT)

Time: Monday 17:45–19:15 Location: H 1012

O 21.1 Mon 17:45 H 1012

Atom-specific spin mapping and buried topological states in a homological series of topological insulators — Sergey V. Eremeev[1,2], Gabriel Landolt[3,4], Tatiana V. Menshchikova[1,2], Bartosz Slomski[3,4], Yury M. Koroteev[1,2], Ziya S. Aliev[5], Mahammad B. Babanly[5], •Jürgen Henk[6], Arthur Ernst[6], Luc Patthey[4], Andreas Eich[7], Alexander A. Khajetoorians[7], Julian Hagemeister[7], Oswald Pietzsch[7], Jens Wiebe[7], Roland Wiesendanger[7], Pedro M. Echenique[2], Stepan S. Tsirkin[1,2], Imamaddin R. Amiraslanov[8], J. Hugo Dil[3,4], and Evgueni V. Chulkov[2] — [1]Tomsk State University, Russian Federation — [2]Donostia International Physics Center, San Sebastián, Spain — [3]Universität Zürich, Switzerland — [4]Paul-Scherrer-Institut, Villigen, Switzerland — [5]Baku State University, Azerbaijan — [6]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [7]Universität Hamburg, Germany — [8]Azerbaijan National Academy of Science, Baku, Azerbaijan

By *ab-initio* calculations and spin-resolved photoemission experiments we demonstrate that a homological series of topological insulators—the binary chalcogenides Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 with the addition of a group IV element—can be tuned in such a way that ideal and isolated Dirac cones are located within the topological transport regime [1]. These compounds exhibit exotic buried topological states strongly protected against surface perturbations and with complex spin textures.

[1] S. V. Eremeev *et al*, Nature Comm. (2011), in press.

O 21.2 Mon 18:00 H 1012

In-plane anisotropy of Fe atoms on Bi_2Se_3(111) — J. Honolka[1], A. A. Khajetoorians[2], V. Sessi[3], T. O. Wehling[4], S. Stepanow[1], J. Mi[5], B. B. Iversen[5], •T. Schlenk[2], J. Wiebe[2], N. Brookes[3], A. I. Lichtenstein[4], P. Hofmann[5], K. Kern[1], and R. Wiesendanger[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Institute for Applied Physics, Universität Hamburg, D-20355 Hamburg, Germany — [3]ESRF, Grenoble, France — [4]1. Institut für Theoretische Physik I, Universität Hamburg, D-20355 Hamburg, Germany — [5]Interdisciplinary Nanoscience Center, Aarhus University, Denmark

Topological insulators exhibit a linearly dispersing gapless topological surface state where both the spin and momentum degrees of freedom are locked. The topological nature of this state results in interesting effects such as suppression of back-scattering. Recently, the robustness of these surface states against magnetic order has been investigated intensively. Here, we explore the magnetic properties of single Fe adatoms on the Bi_2Se_3 surface, in the coverage range $< 1\%$, with combined non-local x-ray magnetic circular dichroism techniques and local low temperature scanning tunneling spectroscopy. We show that the Fe adatoms relax into the surface and exhibit a magnetic easy axis within the surface-plane, contrary to recent reports. Futhermore, we show how *ab-initio* approaches can give a reorientation of the easy axis from out-of-plane to in-plane when considering the interplay of Coulomb interactions, spin orbit coupling, and dynamic hybridization effects.

O 21.3 Mon 18:15 H 1012

Ab initio study of Rashba splitting of 2DEG at the surfaces of topological insulators — Sergey V. Eremeev[1,2], •Maia G. Vergniory[3,4], Tatiana V. Menshchikova[2], and Evgueni V. Chulkov[4,5,6] — [1]Institue of Strength and Materials Science, Tomsk, Russia — [2]Tomsk State University, Tomsk, Russia — [3]Max Planck Institute of Microstructure Physics, Halle, Germany — [4]Donostia International Physics Center, Donostia, Spain — [5]Departamento de Fisica de Materiales UPV/EHU, Donostia, Spain — [6]Centro de Fisica de Materiales CFM-MPC and Centro Mixto CSIC-UPV/EHU, Donostia, Spain

The surface of three dimensional topological insulators (TI) holds a metallic surface state (SS) with Dirac dispersion. Recently it has been demonstrated by using Angle Resolved Photoemission Spectroscopy (ARPES) that besides de Dirac cone 2D electron gas (2DEG) arise at the surface of Bi2Se3 and Bi2Te3 after a few hours of exposition in vacuum or upon deposition of atoms. In this work by means of DFT ab initio calculations we present a new interpretation for the driving mechanism of the simultaneous formation and evolution of the parabolic and M-shaped 2D electron gas (2DEG) bands at the surface of Topological Insulators. As it has been probed in previous publications [7,8] it might be due to an expansion of the van der Waals spacing produced by impurities intercalation. We will show the effect of these expansions on the spatial relocalization of the Dirac cone and we will compare our results with some experimental data for different binary and ternary compounds.

O 21.4 Mon 18:30 H 1012

Reactive chemical doping of the Bi_2Se_3 topological insulator — •Hadj Mohamed Benia, Chengtian Lin, Klaus Kern, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

We studied the evolution of the surface electronic structure of the topological insulator Bi_2Se_3 as a function of water vapor exposure using angle resolved photoemission spectroscopy. We find that a surface reaction with water induces a band bending, which shifts the Dirac point deep into the occupied states and creates quantum well states with a strong Rashba-type splitting. The surface is thus not chemically inert, but the topological state remains protected. The band bending is traced back to Se-abstraction leaving positively charged vacancies at the surface. Due to the presence of water vapor, a similar effect takes place when Bi_2Se_3 crystals are left in vacuum or cleaved in air, which likely explains the aging effect observed in the Bi_2Se_3 band structure.

O 21.5 Mon 18:45 H 1012

Unoccupied electronic states of topological insulators — •Christian Langenkämper[1], Anna Zumbülte[1], Sune N. P. Wissing[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Richard C. Hatch[3], Philip Hofmann[3], Kenta Kuroda[4], Koji Miyamoto[5], and Akio Kimura[4] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany — [3]Department of Physics and Astronomy, Aarhus University, Denmark — [4]Graduate School of Science, Hiroshima University, Japan — [5]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

We report on the first investigation of the unoccupied electronic states of materials which are currently discussed in the context of topological insulators: Bi_2Se_3(111), Sb(111) and $TlBiSe_2$(111). First, different preparation methods (sputter-annealing, cleaving with scotch-tape) will be compared with regard to the surface quality of the samples, i.e. crystallographic order and chemical composition. Second, spin-resolved inverse-photoemission data will be presented. The experimental requirements concerning energy and momentum resolution will be addressed. Our first results show predominantly bulk-derived features with only small spin asymmetries. The experimental data will be discussed along with theoretical calculations for the unoccupied states.

O 21.6 Mon 19:00 H 1012

Quantization of conduction and valence band states through adsorption of nonmagnetic impurities on Bi_2Se_3 — •Marco Bianchi[1], Richard Hatch[1], Zakaria Abd El-Fattah[3], Jianli Mi[2], Bo Brummerstedt Iversen[2], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [2]Departamento de Física de Materiales CSIC-UPV/EHU-Materials Physics Center, E-20018 Donostia-San Sebastián, Spain — [3]Center for Materials Crystallography, Department of Chemistry, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Angle-resolved photoemission (ARPES) can give detailed information on the surface electronic structure of materials. Here we present an ARPES study of the adsorption-induced changes in the electronic structure of the topological insulator Bi_2Se_3(111). Exposure to CO results in strong shifts of the features observed by ARPES. The spectral changes can be explained by a simultaneous confinement of the bulk conduction band and valence band states. This is only possible because of the unusual bulk electronic structure of Bi_2Se_3. The valence band quantization leads to spectral features which resemble those of a band gap opening at the Dirac point. Similar effects are observed

when Rb is adsorbed on the surface. In this case up to seven quantum well states are found in the valence band, both above and below the Dirac point.