# Posters (in alphabetical order, part 1)

### Interfacing Topological Insulators with Magnetic Adlayers: $Fe_3O_4$ on $Bi_2Te_3$

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A gap opening at the Dirac point is predicted for topological insulators in the presence of a disorder potential that violates the time reversal symmetry. This can lead to many interesting novel phenomena, such as the quantum anomalous Hall effect. A breaking of the time reversal symmetry can be realized, for example, by introducing magnetic order. There are two experimental approaches: doping the topological insulator material with transition metal elements or interfacing the topological insulator with a layer of a magnetic insulator. To avoid effects of a non-uniform distribution of the doped elements, we follow the latter approach, and study the effect of a magnetic adlayer.

In our previous work, we have successfully prepared  $Bi_2Te_3$  films by molecular beam epitaxy with high purity and surface cleanliness [1]. This allows us to measure directly the conductivity of the topological surface states [1], and to cap and protect them without affecting their dispersions nor their charge filling [2]. In the next step we are taking up the challenge to prepare ultra clean interfaces of this type of topological insulators with magnetic layers and to measure their properties. Hereby we make use of our expertise of growing high quality films of Fe<sub>3</sub>O<sub>4</sub> [3-5], and interface the well-defined  $Bi_2Te_3$  films with these ferrimagnetic films. We present our study on the growth of Fe<sub>3</sub>O<sub>4</sub> on  $Bi_2Te_3$  and the emerging changes in electronic structure and transport properties.

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# Electrical skyrmion detection with the use of threedimensional topological insulators

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In this work, we investigate the potential of using a three-dimensional topological insulator-ferromagnetic bilayer system as an electrical skyrmion detector. The surface states of the topological insulator interact with the skyrmion magnetization texture via proximity-induced exchange interaction. The co-action of both out-of-plane and in-plane components of the skyrmion with the spin-momentum locked surface states gives rise to a distinct transmission probability than that of the case of a trivial out-of-plane magnetization. Consquently, a change in the conductance can be observed.



Figure : Relative change in conductance when a skyrmion is present with respect to the ferromagnetic texture

### Magnetic topological materials

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While magnetism is usually detrimental to the topological properties, we show that exchange interactions in two-dimensional (2D) topological insulators (TIs) or topological crystalline insulators (TCIs) offer the possibility to realize a variety of new phases depending on the structural symmetry and the direction of the magnetic (exchange) field. For the example of a PbTe monolayer (with mirror and inversion symmetry) a B-field perpendicular to the layer drives a transition from a TCI to a quantum anomalous Hall insulator (QAHI) state [1] with Chern number C=2, while in the non-inversion symmetric Na<sub>3</sub>Bi layer (being both a TI and TCI [2]) only a tilted B-field leads to a QAHI with C=1. Using the concept of the mixed Berry curvature [3], new states like the mixed nodal-line semimetal or the mixed Weyl semimetal can be found in these 2D materials. We also propose magnetic 2D materials that are realizations of these mixed topological phases. They show interesting magnetoelectric coupling phenomena as a function of the magnetization direction. Finally, we also discuss briefly the consequences of antiferromagnetic coupling in these 2D TIs.

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### Magnetic field driven metal insulator transition in Bi<sub>2</sub>Te<sub>2</sub>Se topological insulators

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#### Abstract

Topological insulators (TIs) are a new phase of matter with bulk insulating and conducting surface states. In three dimensional topological insulators such as Bi<sub>2</sub>Se<sub>3</sub>, large numbers of selenium vacancies push the Fermi level inside the conduction band; due to which the charge transport is generally dominated by the bulk current in this crystal and the as grown crystals of Bi<sub>2</sub>Te<sub>3</sub> are p-type because of Te-Bi exchange defects. In order, to extract the surface properties of topological insulators, it is necessary to have insulating bulk state in the TI material. Thus, among the known topological insulators, Bi<sub>2</sub>Te<sub>2</sub>Se with basic quintuple layer as Te-Bi-Se-Bi-Te, emerged as a promising material for studying the topological insulating properties. Bi<sub>2</sub>Te<sub>2</sub>Se is the hybrid material in which the selenium ion occupies the innermost layer in each quintuplet. This will suppress both vacancy formation and Te-Bi exchange defects.

In this work we present our results on  $Bi_2Te_2Se$  (BTS) single crystals grown using modified Bridgeman technique. The R-T behavior of BTS shows a magnetic field driven metal insulator transition. The results reveal a conventional temperature dependence metallic behavior at high temperature (i.e. above 250 K) under applied magnetic field and insulating behavior at low temperatures. A sharp drop in resistance is observed in BTS crystals at zero magnetic field due to weak antilocalization (WAL) effect, which arises from quantum interfering nature of topological insulators. The devices were fabricated (using mechanical exfoliation technique) to investigate the effect of WAL arising from topological surface states. The WAL coefficient of conductance can be tuned by gate voltage and separated in to coherently independent channels, which in topological insulators include both the bulk conduction and topological surface conduction.



Fig.1. (a) Shows the  $R_{xx}$  variation with temperature in the range 2 K  $\leq$  T  $\leq$  350 K with magnetic field. (b) Shows the magneto-resistance behavior at 2 K with clear weak antilocalization effect is observed at zero magnetic field.

### Yu-Shiba-Rusinov states in magnetic Josephson junctions

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Superconductivity and ferromagnetism are two nominally antagonistic states of matter, which lead to extraordinary physical phenomena when combined in one system. Perhaps most striking is the emergence of  $0-\pi$  transitions in magnetic Josephson junctions. We study the bound state spectrum in S/FI/S Josephson junctions in which the ferromagnetic insulator (FI) interlayer introduces scalar and magnetic tunneling. In addition to Andreev-like subgap states, stemming from the coherent coupling of the superconductors (S), magnetic tunneling gives rise to superimposed Yu-Shiba-Rusinov (YSR)-like states. We show that these states have genuine features, which can be tuned by changing the junction characteristics and allow to clearly identify the states in STM experiments. Particularly interesting are zero-energy YSR-like states in the center of the superconducting gap, which form for a wide range of accessible junction configurations. By calculating the Josephson current flow across the system from the spectrum, we unravel a unique connection between these zero-energy YSR-like states and the appearance of  $0-\pi$  transitions in the current flow. Our findings shed new light on the physics of  $0-\pi$  transitions in S/FI/S Josephson junctions.

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# Transport properties of Coulomb blockaded T-junctions

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We investigate the electron transport through a T-shaped junction hosting Majorana bound states (MBS). In particular we consider a Coulomb blockaded T-junction. When the T-junction is in the topologically nontrivial regime it hosts three MBS, localized at the ends of the junction, while there will be one MBS localized at the crossing point of the junction. When the length of the wires are made finite the MBS localized at the ends of the junction overlap with the MBS at the crossing point. We obtain the results of the different transport processes due to the MBS arising in the T-junction in the framework of a master equation where the tunneling Hamiltonian is taken into account in a peturbative manner.

# Estimation of the Dirac point band gap in topological insulators doped with the transition and rare-earth metals

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In recent years numerous of works have been devoted to studying of magnetically doped topological insulators (TIs) due to emergence of the quantum anomalous Hall effect (QAHE). Realization of the QAHE is required opening of the magnetically induced band gap at the Fermi level with formation of the chiral edge states inside this gap. Although, general mechanism of transition to state of the QAHE is well described, proper understanding and controlling of the influence of magnetic dopant on emergence of the QAHE are assumed feather systematic investigation. [1] In the present work we gave attention to the such one main aspect of realization of the QAHE as the Dirac point band gap opening. With this intention we explored electronic structure of the Dirac cone and magnetic properties in  $Bi_{(2-x)}Te_z Se_{(3-z)}$  doped with transition metals (TM):  $Mn_{(x=0.3)}, V_{(x=0.06)}$  and in  $Bi_{(2-x-y)}Sb_yTe_3$  doped with rare-earth metals (REM):  $Dy_{(x=0.06)}, Gd_{(x=0.06)}, Er_{(x=0.06)}$ . We applied different concentration of Sb and Se atoms in the samples for shifting position (in energy) of the Dirac point and uncrossing it with the Fermi level. That affords ground for the band gap analyzing. Dopants we studied possess different magnetic moment from the low for Er to the highest for Gd, which can be applied for gently variation of internal magnetic moment and induced band gap. It is believed that doping of TIs with REM is more beneficial since magnetic TM are usually divalent and act also as electric dopants. [2] REM (Gd, Er, Dy) are trivalent and has an equal number of bonding electrons to Bi (Sb), therefore, only magnetic moment can be induced.

For analysis of the samples we have used several methods such as angular resolved photoemission spectroscopy (ARPES), resonance PES and Superconducting Quantum Interference Device (SQUID). ARPES with high resolution has been applied for the band gap and the Dirac cone shifting investigations. For the following treatment we have used approach with modeling of experimental spectra. It allows to reduce features appeared during measurements and make more correct estimation of the band gap. Resonant PES has been used to match the location and contribution of the bands of the magnetic impurities in PES spectra hereby has given information of their bonding with atoms of TI. Finally, direct magnetic measurements have been carried out by SQUID.

Based on these experimental measurements we have examined origin of the band gap opening in magnetically doped TIs. Either we will show changing of the band gap related to the element of magnetic impurity. As one of the way of the Dirac point gap modification role of the 2D surface Dirac-fermion-mediated magnetic coupling will be discussed. Moreover, the Dirac cone shifting under various energies of photos will be analyzed in REM doped TIs as it previously has been done for pristine and V doped TIs. [3]

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# Visualizing a nematic domain wall in bismuth: a tunable platform for topological edge modes

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Gapless edge modes are often realized at boundaries between topologically distinct phases. These can occur not only at physical edges of a system, but also at interfaces within a sample, such as domain walls between different broken symmetry phases. In this talk, I will describe scanning tunneling microscope measurements that allow us to locally probe a nematic domain wall and its edge excitations on the surface of bismuth. The valley degeneracy in this material is lifted at high field to produce nematic quantum Hall states with broken rotational symmetry. By directly imaging the resulting anisotropic Landau level wave functions, we detect an abrupt switch in valley occupation across the domain wall. Spatially resolved spectroscopy shows enhanced low-energy differential conductance at the boundary and matches well to theoretical modeling, which predicts counter-propagating valley-polarized edge states. Moreover, by tuning Landau level filling, we can change the number of modes at the interface, which affects the degree of inter-valley scattering and hybridization of the one-dimensional states.



# Contribution submission for NTTI 2018 Title: Fundamental limits to helical edge conductivity due to spin-phonon scattering

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We study theoretically the effect of electron-phonon scattering in 2D topological insulator (2DTI) edge states. Due to the spin-momentum locking in helical edge states, dynamical deformations of the edge modify the spin texture of the electronic edge states. In our work, we show that the resulting spin-phonon coupling ultimately leads to backscattering.

For a short channel, we compute the temperature-dependent conductance in the linear regime  $(\beta eV < k_BT)$  using the Kubo formula, and find  $\delta G \propto T^5$  for the backscattering conductance. In the limit of a long edge channel, transport becomes diffusive and we compute the resistivity  $\rho$  using the semi-classical Boltzmann equation. In particular we find a metallic Bloch-Grüneisen behaviour for chemical potentials near the Dirac point.

Since this spin-phonon coupling arises even in ideal samples and since further imperfections (e.g. Rashba impurities, charge puddles, electron-electron interactions etc.) can only increase backscattering, our results impose a fundamental upper limit on the conductivity of 2D TI edge states.

# Transport properties of $Pb(Bi_{1-x}Sb_x)_2Te_4$ Topological Insulators

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Existence of topological surface states in  $PbBi_2Te_4$  series materials was first verified by Souma et al. [1] and Kuroda et al. [2] independently using ARPES technique. Souma et al. also reported that by controlling Sb doping ratio, Fermi level can be tuned. However, bulk insulating samples have never been obtained in this material. In view of this, we fabricated a series of  $Pb(Bi_{1-x}Sb_x)_2Te_4$  and systematically studied the transport properties in order to enhance bulk resistivity of this series and also to clarify the conduction mechanism.

A series of  $Pb(Bi_{1-x}Sb_x)_2Te_4$  topological-insulator crystals with various Sb molar ratios x was fabricated by vertical Bridgman method. Resistivity was measured in the temperature range 2-300 K. Magnetoresistance was measured at various temperatures in the magnetic field up to 9 T.

The results are shown in Figs. 1 and 2. Precise control of Sb concentration made it possible to fabricate bulk insulating samples for the first time in this system [3](Fig. 1). In the low temperature region, temperature and magnetic field dependences of resistivity agree well with a 3D WAL-WL model[4]. In this talk, we will further discuss the conduction mechanism in the bulk insulating samples in relation to an impurity band formed within the bandgap.



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## Temperature dependent spin polarization in EuO thin films investigated by high resolution ARPES

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The ferromagnetic insulator EuO is predicted to show 100% spin polarization at the valence band maximum, which makes this material a prototype candidate for research in the field of spintronics. Our goal is to interface it with a topological insulator to introduce time-reversal symmetry breaking without an external magnetic field.

As a first approach we studied MBE growth of EuO on Cu(001), because Cu is a very good electrical conductor, thus, ideally suited as an aid for charging problems in band mapping from an insulating thin film. After we could narrow down the EuO synthesis to a very small parameter window, in which single-crystalline growth is mastered, we performed temperature dependent high resolution spin-ARPES measurements. A non-vanishing spin polarization of the O 2p band due to exchange splitting as well as up to 52% in the Eu 4f band could be obtained. Furthermore, the temperature dependence of the Eu 4f polarization can be described by the Brillouin function and confirms the literature value of  $T_C = 69$  K.

### High throughput screening for 2D and 3D topological materials

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Topological insulators (TIs), with insulating band gaps and nontrivial edge states, have been widely investigated not only for their fundamental importance but also owing to their potential applications [1]. The current bottleneck is to identify better topologically nontrivial materials which can be integrated into devices more feasibly, and previous efforts have relied mostly on trial-and-error procedures or chemical/physical intuition. To search for two-dimensional (2D) and three-dimensional (3D) TIs, we developed a high throughput framework which can be utilized to screen materials with only crystal structures as inputs. The methodology is implemented based on the automated construction of maximally localized Wannier functions using a poor-man?s algorithm, where the partial density of states from the first principles calculations are integrated in order to determine the proper projection and the energy windows. The topological character of the band gaps is determined by the calculations of the surface states for semi-infinite slabs/ribbons. To further confirm the nontrivial nature of the band gaps for the possible candidates, appropriate topological invariants, such as Z2 number, mirror Chern number, etc., are evaluated based on the density functional theory electronic structure, together with Wannier centers. We have applied our methods to both 2D monolayers from the 2D materials database [2] and 3D ternary nitrides and Bi- and Sb-based compounds from the Materials Project database [3]. From 746 2D material candidates and 3782 3D ternary compounds, we have successfully identified four 2D TIs and seven new 3D TIs, whose topological properties will be discussed in detail.

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### Dephasing in Mach-Zehnder interferometer by an Ohmic contact

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We study dephasing in an electronic Mach-Zehnder (MZ) interferometer based on quantum Hall (QH) edge states by a micrometer-sized Ohmic contact embedded in one of its arms. We find that at the filling factor  $\nu = 1$ , as well as in the case where an Ohmic contact is connected to an MZ interferometer by a quantum point contact (QPC) that transmits only one electron channel, the phase coherence may not be fully suppressed. Namely, if the voltage bias  $\Delta \mu$  and the temperature T are small compared to the charging energy of the Ohmic contact  $E_C$ , the free fermion picture is manifested, and the visibility saturates at its maximum value. At large biases,  $\Delta \mu \gg E_C$ , the visibility decays in a power-law manner.

## Observation of the unoccupied state of SnTe by laser-excited angle resolved photoemission spectroscopy

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Topological crystalline insulator (TCI) is a novel class of topological insulators (TIs), in which topological surface state (TSS) is protected by the mirror symmetry of the crystal[1], instead of the time-reversal symmetry in the conventional  $Z_2$  TIs. SnTe is a typical material of TCIs with the topological protection due to the mirror reflection symmetry with respect to the six {110} planes of the rock salt crystal structure. Experimentally, the TSSs of SnTe were observed by angle-resolved photoemission spectroscope (ARPES) measurement on the (100) and (111) surfaces. However, the observation was limited only to a lower-part of the surface band below the Fermi energy  $E_F$ , which is located below the top of valence band (VB), due to a strong tendency of actual crystals being p-type degenerate[2]. In the present work, we have attempted to observe the whole structure of the surface band of the SnTe (111) surface using time-resolved (Tr-) ARPES measurement with the excitation by pump and probe pulses.

SnTe thin films were prepared by molecular beam epitaxy (MBE). We grew a SnTe (111) layer on a thick CdTe layer deposited on a p-GaAs(111)A wafer. After the growth, the SnTe thin films were transported to the chamber for the Tr-ARPES measurement using a suitcase chamber without exposed to the air. The Tr-ARPES measurement was carried out using a Ti-sapphire laser system which delivers 1.48 eV pump and 5.92 eV probe pulses at a repetition rate of 250 kHz[3].

Figure 1(a) shows the time-integrated ARPES image around the  $\overline{\Gamma}$  point of the SnTe (111) surface. This image was obtained by integrating Tr-ARPES images in the range of 0 ~ 0.76 ps after the excitation by a pump pulse, which makes it possible to observe the whole band structure including the unoccupied state. As a result, we see clearly the conduction band (CB) and the top of VB above  $E_F$ . It should be noted that the VB exhibits a large Rashba splitting, corresponding to parameter  $\alpha$  of ~4 eVÅ. Such a large Rashba

splitting was also reported in Bi-doped (Pb,Sn)Te[4]. In addition, one can discern a weak trace between the CB and VB, corresponding to the surface state. As shown clearly in the momentum distribution curves (MDCs) (Fig. 1(b)), this surface band exhibits a linear dispersion, consisting of two lines which crosses at around  $E-E_F = 0.2$  eV and their spacing increases with energy. This shape and position of the surface band is different from a previous report[2], in which the surface band was presumed by extrapolating the observed state below  $E_F$ . Details will be discussed at the conference.



Fig. 1(a) Time-integrated Tr-ARPES image recorded around  $\overline{\Gamma}$  point of the SnTe (111) surface. (b) MDC plots at different binding energies extracted from (a)

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### Delocalized Shiba bands in magnetic clusters at superconducting surfaces

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If a number of magnetic adatoms is placed sufficiently close to each other on the surface of a superconductor, their Shiba states hybridize and form a band structure inside the superconducting gap. For multiple magnetic adatoms (clusters) with equal distances between them, we demonstrate the formation of delocalized, effectively spin-unpolarized Shiba states with energies independent of the spin structure of the cluster. We solve the problem analytically and analyze both spin-polarized (dispersive energy levels) and spin-unpolarized (pinned energy levels) solutions. The wave functions of the spin-unpolarized solutions effectively decouple from the net magnetic moment of the cluster. For this reason, they form the pinned energy bands, which make them stable against thermal fluctuation and detectable in STM experiments. The energies of the spin-polarized solutions can be characterized solely by the net magnetic moment of the cluster.