Contributed talks
(in alphabetical order)

2-dimensional superconductivity in SnTe on Bi/Si(111)

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SnTe is one of typical materials in topological crystalline insulators, TCIs. SnTe has been investigated originally as a narrow-gap band-inversion semiconductor which has a energy gap of 0.2 eV before being recognized as a TCI. Transport characteristics relating to the topological surface states have been reported so far by demonstrating quantum interference phenomena such as weak antilocalization in thin films [1,2] and Shubnikov-de Haas oscillations in nanowires [3]. In addition, ARPES measurements also have revealed the surface-state bands these days. On the other hand, topological superconductivity attracts much attention because it shows abundant exotic properties as shown in Cu intercalated Bi_2Se_3 such as Majorana fermion, non-commutative statistics which enables quantum computing. However, confirmation of topological superconductivity (TSC) is still ongoing, and candidates of other materials are required. Especially, since TSC in TCI has been proposed only in $Sn_{1-x}In_xTe$, realizing TSC of TCI is interesting. Although inducing superconductivity in TCI is not sufficient condition for TSC, it is certainly one possibility to realize TSC.

In this study, we aim to induce superconductivity in SnTe without doping. Theory predicts that IV-VI group semiconductors such as PbSe and PbTe can show interface superconductivity due to a partially-filled flat band induced by strain [4]. However, superconductivity using SnTe and investigation with respect to TCI has not been reported. To induce strain, we used Bi(111) as an under-layer which has different lattice constant from SnTe. The lattice parameters of Bi and SnTe are 4.54 and 4.48 Å, respectively, and thus the tensile strain is induced at the interface of SnTe and Bi. In SnTe, with increasing the tensile strain, the Fermi level is raised, leading to the metallic nature. Such a change can induce superconductivity. Figure 1(a) shows the temperature dependence of resistance under some magnetic fields perpendicular to the surface up to 1.0 T. The onset temperature of superconductivity at 0 T is $\sim$ 5.8 K, and it decreases with increasing the magnetic field. Figure 1(b) represents the magnetic field dependence of resistance at some temperatures up to 10 K. The critical magnetic field decreases with increasing temperature. Although resistance does not drop to zero, indicating that superconductivity is partial, the origin may be due to the interface superconductivity as shown in a previous report [5]. This superconductivity was revealed to be two-dimensional characteristics as confirmed by transport measurements with rotating the sample under the magnetic field. We will discuss properties of superconductivity in details in the presentation.

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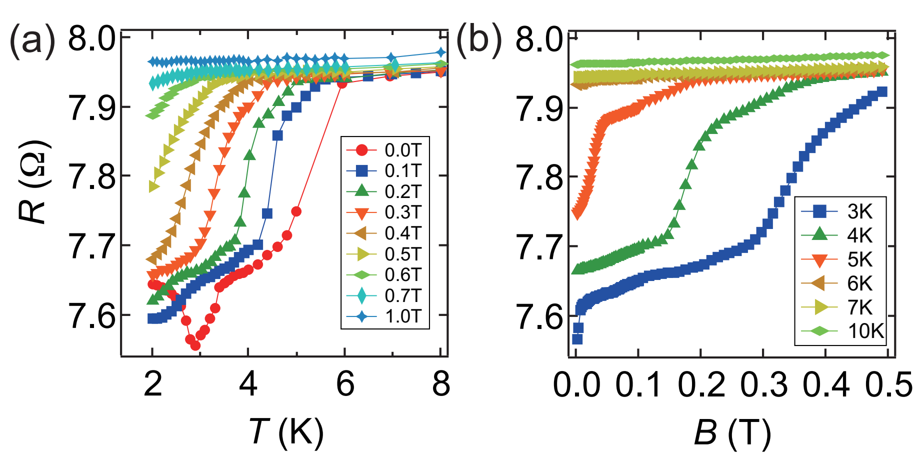

FIG. 1: (a)Temperature dependence of resistance with some applied magnetic fields ranging 0 - 1.0 T. (b) Magnetic fields dependence of resistance at some temperatures ranging 3 - 10 K

$\mathbb{Z}_4$ parafermions in one-dimensional fermionic lattices

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Parafermions are emergent excitations which generalize Majorana fermions and are potentially relevant to topological quantum information. Using the concept of Fock parafermions, we present a mapping between lattice $\mathbb{Z}_4$ parafermions and lattice spin-1/2 fermions which preserves the locality of operators with $\mathbb{Z}_4$ symmetry. We use this to construct a one-dimensional fermionic Hamiltonian which hosts exact parafermionic edge states. We discuss their protection against various perturbations as well as their visibility in the fermionic spectral function.

Isotropic and anisosotropic transport properties of the Weyl semimetal type-II WTe_2

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Because of the nearly perfect compensation of electrons and holes, the Weyl semimetal type-II WTe_2 exhibits a giant quadratic magnetoresistance, with no saturation observed even at very high magnetic field [1]. According to a simple two bands model, the magnetoresistance curvature d^2R/dB^2 is given by the transport mobility of the charge carriers. Whereas the absence of magnetoresistance saturation was reported in many experiments so far and appears to be therefore a common property, the curvature of the magnetoresistance strongly depends on the device and can vary by almost 5 orders of magnitudes [2,3]. This curvature is generally large in macroscopic crystals of good quality and vanishes in exfoliated nanostructures [3]. The control of the transport mobility and more generally the understanding of the interactions between charge carriers and a static disorder in WTe_2 is therefore a key issue if we want to control and increase the magnetoresistance in such devices.

In the present work, we investigate the transport properties of a WTe_2 flake studied at very low temperature (down to 100 mK) and under magnetic field (up to 6 T). The densities and transport mobilities are extracted for electrons and holes by measuring longitudinal and Hall resistances as well as Shubnikov-de Haas oscillations. According to the Hall and longitundinal voltage measurements, the crystal is found to be charge compensated within about 1%. This is confirmed by the direct observation of Shubnikov-de Haas measurements for both holes and electrons. Although the transport properties are isotropic, we show that the scattering is anisotropic, which reveals a long-range disorder. A theoretical model allow us to extract the correlation length of the disorder and points at some fundamental limitation to improve the transport mobility of type-II Weyl semimetals.

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Majorana Corner Modes in a Second-Order Kitaev Spin Liquid

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Higher-order topological insulators are distinguished by the existence of topologically protected modes with codimension two or higher. In this talk, I will present a manifestation of second-order topological insulators in a 2D frustrated quantum magnet, which exhibits topological corner modes. Our exactly-solvable model, a generalization of the Kitaev honeycomb model to the Shastry-Sutherland lattice, exhibits a gapped spin liquid with Majorana corner modes protected by two mirror symmetries. This second-order Kitaev spin liquid remains stable in the presence of thermal fluctuations and undergoes a finite-temperature phase transition evidenced in large-scale quantum Monte Carlo simulations.

Transport properties of topological insulators with Z_2 indices of (1;111)

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Most of the topological insulators (TIs) found so far, including most-intensively studied $(\mathrm{Bi,Sb})_2(\mathrm{S,Se,Te})_3$ tetradymites, have the Z_2 indices of (1;000). In the present study, we investigate transport properties of the TIs of Bi-Sb and $\mathrm{Pb(Bi,Sb)_2Te_4}$, both of which have the indices of (1;111). According to the classification by Slager et al.[1], TIs with (1;111) belong to the class of " translationally active " states, in which 1D gapless states can form along crystalline dislocations[1][2]. In contrast, in TIs with (1;000), no such states can be realized.

For Bi-Sb, high-density well-aligned dislocations were introduced by plastic deformation. FIG.1 shows temperature dependences of electrical resistivity along different directions, which are parallel (R_{para}) and perpendicular (R_{perp}) to the dislocation line direction. We can see a considerable difference between the two directions below 50K: R_{para} is much reduced compared to R_{perp}. A quantitative analysis showed that the reduction in resistivity can reasonably be attributed to dislocation conduction [3].

On the other hand, for $\mathrm{Pb(Bi_{1-x}Sb_x)_2Te_4}$, we conducted a systematic study of their transport properties, aiming at realizing enhanced bulk insulation in this system [4]. Hall-effect measurements showed that n- to p-type transition in bulk conduction occurred at x=0.8. Semiconducting behavior with a negative temperature coefficient of resistivity was observed with resistivity values as high as 180 mΩcm at 2K around the transition composition, as shown in FIG. 2.

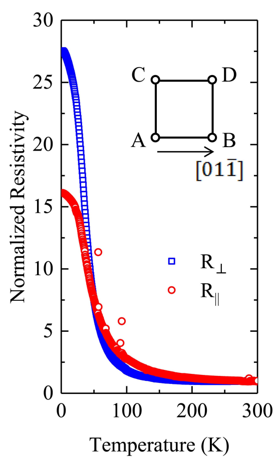

FIG. 1: Normalized resistivities for R_{para}(red) and R_{perp}(blue)

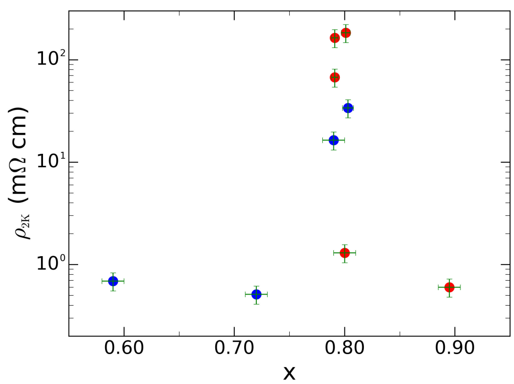

FIG. 2: Resistivity at 2 K (ρ_{2K}) plotted against the x values evaluated by EPMA, where the blue and red circles are assigned to the negative and positive carrier types, respectively

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Fluctuation-induced magnetic skyrmions at topological insulator surfaces

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Ferromagnets in contact with a topological insulator have become appealing candidates for spintronics due to the Dirac surface states, which exhibit spin-momentum locking. Bilayer Bi_2Se_3-EuS structures, for instance, show a finite magnetization at the interface at temperatures well exceeding the Curie temperature of bulk EuS. Here we determine theoretically the effective magnetic interactions at a topological insulator-ferromagnet interface {\it above} the magnetic ordering temperature. We show that by integrating out the Dirac fermion fluctuations an effective Dzyaloshinskii-Moriya interaction and magnetic charging interaction emerge. As a result individual magnetic skyrmions and extended skyrmion lattices can form at interfaces of ferromagnets and topological insulators, the first indications of which have been very recently observed experimentally.

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Type-I and type-II classification of composite Weyl nodes

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Weyl nodes with chiral charge $\chi = \pm 1$ are classified in type-I and type-II according to the tilting of conical band dispersion around the band degeneracy. The Fermi surface, which is described by a 2^{nd} order algebraic surface, is different for each type of band crossing. In the case of type-I, the Fermi surface consists of a closed hole(electron) pocket that collapses into a single point at the energy of the Weyl point, and reemerges as an electron(hole) pocket. On the contrary, a type-II Weyl point produces Fermi surface composed of two open sheets, that correspond to an electron and a hole pockets, and undergo a Lifshitz transition at the energy of the Weyl point. In this work, we show that this simple classification is enlarged for the case of composite Weyl nodes. When the C_4 and C_6 rotation symmetries forbid linear dispersion of the energy around the band touching point on the plane perpendicular to the symmetry axis, as it happens in the composite Weyl nodes, terms with a quadratic or cubic dispersion must be included into the Hamiltonian. Consequently, the Fermi surface produced by the quadratic or cubic energy dispersion is described by a 4^{th} or 6^{th} order algebraic surface, respectively. We can still classify the composite Weyl nodes in two different types (I and II) according to the relation between the kinetic and potential components of the energy spectrum. However, each type of crossing can exhibit a Fermi surface with different new morphologies. For example, we show that it is possible to have a band degeneracy with a new type of Fermi surface morphology. At a chemical potential μ below(above) the Weyl node, the Fermi surface is comprised of several open sheets. When μ is at the energy of the Weyl point, the open Fermi sheets touch each other at a single point. Increasing (decreasing) the chemical potential, the open Fermi sheets split again and a closed sheet emerges from the band degeneracy point. In this work we present the different morphologies that we have found for the composite Weyl nodes, and illustrate some of them in real materials such as bcc iron.

Electrical Conductions along Dislocations in Bismuth-Antimony Topological Insulators

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In 2009, it was theoretically predicted that topologically protected metallic states form along dislocations in three dimensional (3D) topological insulators (TIs) when a specific condition is satisfied [1]. Though such metallic dislocations in TIs have a potential for novel applications as robust quantum nanowires, no experimental works had been reported until very recently; we reported in a previous paper [2] that conductivity measurements on plastically deformed Bi-Sb TIs showed excess conductivity owing to dislocation conduction. However, in the measurements, millimeter-sized specimens were used, in which dislocations did not penetrate the sample completely. As a result, the ratio of the dislocation conductance to the bulk one was fairly small, hampering further detailed studies of dislocation conduction. In the present study, we carried out the resistivity measurements for micrometer-sized specimens of deformed Bi-Sb alloys, in which dislocations should penetrate the sample.

Bi-Sb single crystals were grown under a controlled temperature. Electron probe microanalyses showed the compositions of the grown crystals to be $Bi_{1-x}Sb_x$ (x$\simeq$0.15), which were within the insulating regime of $0.07 < x < 0.22$. Rectangular samples were cut out, and uniaxially compressed to introduce dislocations. Transmission electron microscopy (TEM) observations were performed to examine the density, Burgers vector, and configuration of the introduced dislocations.For resistivity measurements, micrometer-sized samples with dimensions $4.3 \times 4.4 \times 13\ \mu m^3$ were cut out by focused ion beam. The resistivity measurements were carried out by a four-probe method in the temperature range 2-300K.

The figure presents the result of the resistivity measurement. The resistivity value at room temperature is about 140 mΩcm, which is much higher than those reported previously for Bi-Sb TIs (<1 mΩcm) [2]. This apparent discrepancy may be related to fluctuation of Sb concentration in the sample. Because Bi-Sb is a solid solution system, concentration fluctuation often occurs in bulk samples. Here, bandgap width, and therefore, the resistivity value varies with the Sb concentration. Then, the concentration fluctuation should suppress the resistivity value because low resistivity portion usually determines the measured value. In contrast, the concentration fluctuation must be severely suppressed for our micrometer-sized sample, which should result in a high resistivity value. Another possibility is that the resistivity has been raised by electron scattering by high-density dislocations.

The temperature dependence of resistivity in the figure is substantially different from those for conventional semi-conductors and also from those previously reported for Bi-Sb TIs in previous works [2]. That is, the resistivity increase with decreasing temperature is not observed in this result. Instead, the resistivity decreases dramatically with decreasing temperature, going down to 2 mΩcm at 2K, which is only 1.4% of the room temperature value. In this talk, we will discuss the origin of this peculiar behavior in light of the dislocation conduction.

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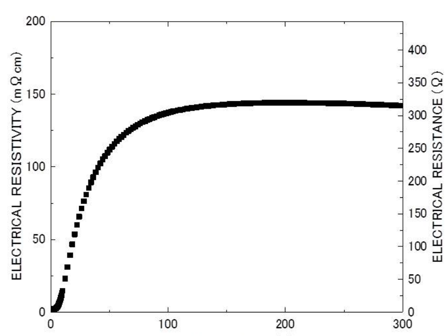

FIG. 1. The result of the resistivity measurement.

Dynamic and e^2/h-quantized photocurrent response in three-dimensional topological insulators

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Topological materials are quantum materials where the electron and spin properties are dominated by topology. Particularly, three-dimensional topological insulators are a class of Dirac materials with two-dimensional metallic surface states featuring spin-momentum locking, i.e., each momentum vector is associated with a spin locked perpendicularly to it in the surface plane. In revealing the optoelectronic dynamics in the whole range from femto- to microseconds, we demonstrate that the long surface lifetime of Bi_2Te_2Se-nanowires allows accessing the respective surface states by a pulsed photoconduction scheme even at room temperature [1]. Moreover, the symmetry of helicity-dependent photocurrents in Bi_2Te_2Se-platelets can be broken by extrinsic and intrinsic anisotropies within the circuits. In particular, we observe a helical, bias-dependent photoconductance at the lateral facets of topological Bi_2Te_2Se-platelets for perpendicular incidence of light, indicative of spin accumulation as induced by a transversal spin Hall effect in the bulk states of the Bi_2Te_2Se-platelets [2].

In addition, we demonstrate a quantized photoconductance of e^2/h at the edges of Bi_2Se_3- and $BiSbSe_3$-circuits at low temperatures, which we can explain by a broken time-reversal symmetry given by the overall electrostatics of the devices [3].

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Relativistic Gurzhi effect in channels of Dirac materials

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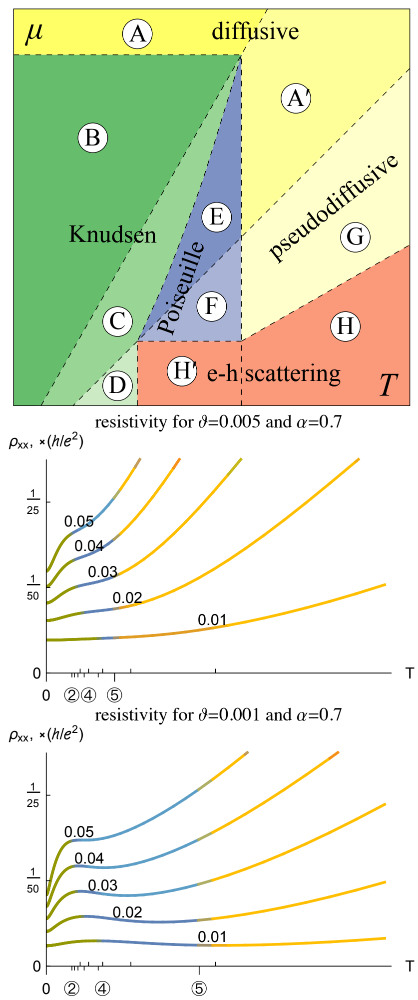
Charge transport in channel-shaped 2D Dirac systems is studied employing the Boltzmann equation. The dependence of the resistivity on temperature and chemical potential is investigated. An accurate understanding of the influence of electron-electron interaction and material disorder allows us to identify a parameter regime, where the system reveals hydrodynamic transport behavior. We point out the conditions for three Dirac fermion specific features: two-liquid hydrodynamics, pseudo-diffusive transport, and the electron-hole scattering dominated regime. It is demonstrated that for clean samples the relativistic Gurzhi effect, a definite indicator of hydrodynamic transport, can be observed.



A New Class of Ferromagnetic Insulator Based on Hetero-Epitaxial $BTO - BFO/LSMO$ Magnetoelectric Composite

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Magnetic insulators are potentially excellent candidates for pure spin current without the existence of charge current. In this scheme, the spin accumulation will interact with the magnetic moments of the insulator layer, resulting in spin torques which can initiate precession and switching[1,2] without the spin-polarized electrons entering the insulator layer[3].

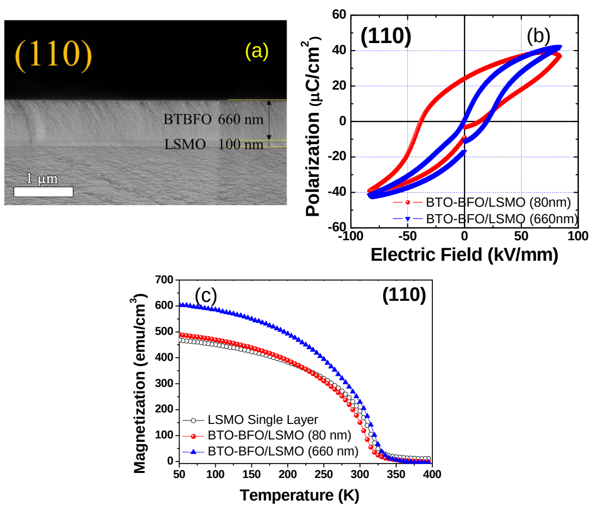

FIG. 1: (a) TEM image of BTO-BFO/LSMO heterostructure. (b) For two different thicknesses of BTO-BFO, the P-E curves of the hetero-epitaxial films, are presented. (c) Temperature dependence of magnetization in the composite films. The magnetization is compared with a LSMO film.

Thin-film magnetic insulator yttrium iron garnet (YIG)[4] has shown sufficiently low damping on the order of 10^{-4}. Other than YIG, there are only limited studies quantifying the Gilbert damping parameter of thin-film magnetic insulators[5,6]. This indicates the challenges in conducting studies on insulating thin-film material.

We synthesized epitaxial BTO-BFO heterostructure with decreased leakage and simultaneously improved the multiferroic properties. We observed small Gilbert damping (α =0.004) and the absence of large inhomogeneous broadening. This fact offers opportunities for employing this material system for spin transfer in multifunctional materials where controlling magnetization by a flow of spin angular momentum, or spin current, is crucial toward developing nanoscale spin-based memory and devices. Figure 1a, shows our hetero-epitaxial BTO-BFO/LSMO thin films grown on (110) oriented $SrTiO_3$ (STO) substrates by off-axis RF magnetron sputtering. Figure 1b and Fig. 1c are examples of the ferro-electric loops and the temperature dependence of magnetization as a function of BTO-BFO layer thickness. This heterostructure can be important for spin transfer in multifunctional materials and this talk will present several important aspects of these materials systems.[7–9]

1. ACKNOWLEDGMENT:

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Photo-induced surface Dirac states of topological insulators

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The surface of topological insulators (TIs) is considered as a promising platform for novel spin-electronic functions. Generating spin-polarized surface currents out of the spin-polarized metallic states would be a milestone function, and optical means provides several pathways to this end. One way is to utilize the surface photovoltage (SPV) effect, as proposed recently [1, 2]. The idea is to shine light in the surface band bending region developed on the edge of so-called bulk-insulating TIs; see Fig. 1. Similar to the generation of photovoltage in solar-cell batteries, voltaic change can be induced on the illuminated area of surface through the SPV effect. Because the surface is intrinsically metallic, surface current will either flow out of or into the illuminated area from the dark surroundings depending on the polarity of the SPV; and because the surface states are spin polarized, the photo-gated surface current will also be spin polarized.

Here, we use time- and angle- solved photoemission spectroscopy (TARPES) implemented by the pump-probe method as a direct access to photo-induced redistribution of electronic band structure and directly observed downward and upward photovoltaic shifts on the *n*- and *p*-type sample surfaces, respectively, and the amount of the shift is controlled by the power of pump. We also observed polarity-dependent changes in the filling of the topological surface states for > 4 μs. The results can be nicely explained by the Schottky barrier junction model. We provide keys, besides the bulk insulation, for TIs to meet the semiconductor-junction functions, and show a way [3] to manipulate the light-induced current on TIs. Furthermore, we observed a 1.7 times larger SPV after the optical aging of the sample. We propose that this result is caused by sharpened band bending [4]. Our findings open an avenue for achieving optical control of spin-polarized current generators by utilizing topological insulators and micro-fabrication techniques to vary the laser spot size to tune the band bending via infrared laser illumination.

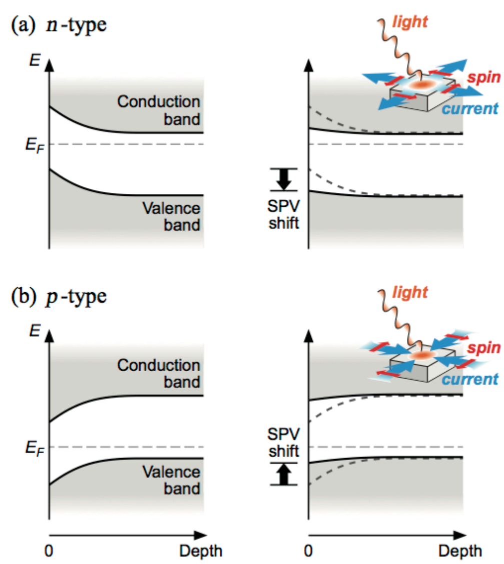

FIG.1: The surface photovoltage effect on TIs. Conduction and valence bands bend on approach to surface in both *n*- (a) and *p*-type (b) TIs, as shown in the left panels. When illuminated, the bending relaxes and photovoltage is generated on surface (right panels). Upper right schematics in the right panels show the flow of spin-polarized current on metallic surface of TIs out of (a) and into (b) the illuminated area.

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Magneto-transport in 3D topological insulator nanowires

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We investigate the transport characteristics of 3D topological insulator (3D TI) nanowires in external electric and magnetic fields. The wires host topologically non-trivial surface states wrapped around an insulating bulk and are modelled by surface effective Hamiltonians. A magnetic field along the wire axis leads to Aharonov-Bohm type oscillations of the conductance. Such oscillations have been observed in numerous systems and signal surface transport, though alone cannot prove its topological nature. Furthermore, it is not known how they are affected by the wire specific geometry which is never perfectly tubular as assumed in theoretical models up to now.

We thus focus on two issues: (i) An accurate modelling of surface transport in gated, strained HgTe nanowires, accompanying experimental measurements performed by our collaborators (J. Ziegler & D. Weiss, Uni Regensburg); (ii) A theoretical study of magneto-conductance through shaped (tapered, curved) 3D TI nanowires. In particular, a non-constant radius along the wire direction gives rise to a spatial variation of the enclosed magnetic flux, implying novel quantum transport phenomena.

Experimental evidence of proximity induced odd-frequency superconductivity in a topological insulator

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At an interface between a topological insulator (TI) and a conventional s-wave superconductor, the induced superconductivity in the TI surface state is expected to develop a complex p-wave order parameter which may allow to create Majorana Fermions inside vortex cores. These collective excitations are their own antiparticles and are the basic element in a proposal for fault-tolerant quantum computing. Here we present experimental evidence for proximity induced superconductivity in a thin layer of the TI Bi_2Se_3 grown on top of Nb. From depth-resolved muon spin rotation measurements in the Meissner state, we observe a local enhancement of the magnetic field in Bi_2Se_3 that exceeds the externally applied field, thus supporting the existence of an intrinsic paramagnetic Meissner effect arising from an odd-frequency superconducting state.

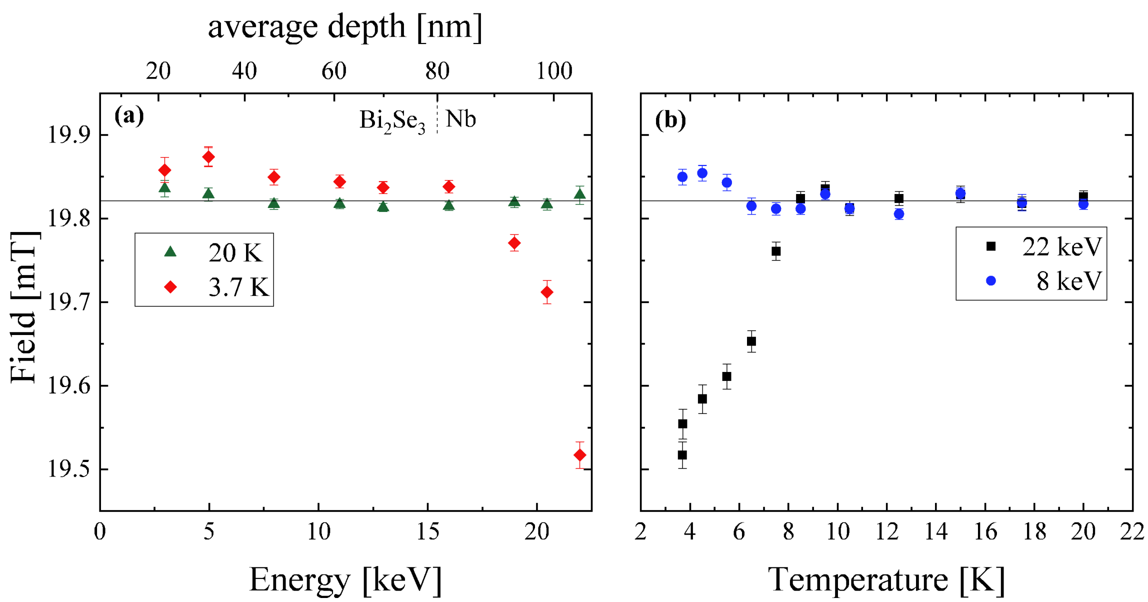

FIG. 1: Implantation energy (a) and temperature (b) dependence of the mean field. The muons implanted at a high energy stop in Nb and see a conventional Meissner screening below 8 K. However, the lower energy muons stopping in Bi_2Se_3 see an increase of the local magnetic field. The solid line shows the energy average of the mean field at 20 K.

Unpaired Weyl nodes from Long-Ranged Interactions: Fate of Quantum Anomalies

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We study the effect of long-ranged interactions on Weyl semimetals. Such interactions can give rise to unpaired Weyl nodes, which we demonstrate by explicitly constructing a system with just a single node – a situation that is fundamentally forbidden by fermion doubling in non-interacting band structures. Adding a magnetic field, we investigate the fate of the chiral anomaly. Remarkably, as long as a system exhibits a single Weyl node in the absence of magnetic fields, arbitrarily weak fields qualitatively restore the lowest Landau level structure of a non-interacting Weyl semimetal. This underlines the universality of the chiral anomaly in the context of Weyl semimetals. We furthermore demonstrate how the topologically protected Fermi-arc surface states are modified by long-ranged interactions.

Designing 3D topological insulators by 2D-Xene (X = Ge, Sn) sheet functionalization in GaGeTe-type structures

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State-of-the-art theoretical studies anticipate a 2D Dirac system in the heavy analogues of graphene, free-standing buckled honeycomb-like Xenes (X = Si, Ge, Sn, Pb, etc.). Herewith we regard a 2D sheet, which structurally and electronically resembles Xenes, in a 3D periodic, rhombohedral structure of layered AXTe (A = Ga, In; X = Ge, Sn) bulk materials. This structural family is predicted to host a 3D strong topological insulator with $\mathbb{Z}_2 = 1;(111)$ as a result of functionalization of the Xene derivative by covalent interactions. The parent structure GaGeTe is a long-known bulk semiconductor; the heavy, isostructural analogues InSnTe and GaSnTe are predicted to be dynamically stable. Spinorbit interaction in InSnTe opens a small topological band gap with inverted gap edges that are mainly composed of the In-5s and Te-5p states. Our simulations classify GaSnTe as a semimetal with topological properties, whereas the verdict for GaGeTe is not conclusive and urges further experimental verification. The AXTe family structures can be regarded as stacks of 2D layered cut-outs from a zincblende-type lattice and are composed of elements that are broadly used in modern semiconductor devices; hence they represent an accessible, attractive alternative for applications in spintronics. The layered nature of AXTe should facilitate the exfoliation of their hextuple layers and manufacture of heterostructures [1].

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Magnetoconductance of multi-terminal 3D topological insulator nanostructures

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We study the magnetoconductance of patterned multi-terminal nanostructures of 3D topological insulator (TI) materials such as Bi_2Se_3, for which a fabrication method was recently developed (see Fig. 1 (b-c) and [1]). We make use of the effective 4-band tight-binding Hamiltonian, based on the continuous model developed by Zhang *et al.* [2], to perform ballistic transport simulations with a parallelized implementation of the software package Kwant. Our results show that, similar to straight 3D TI nanowires, a robust gapless helical subband can be obtained in these nanostructures when they are pierced by a half-integer magnetic quantum flux but, unlike for straight wires, the direction and perpendicular component of the magnetic field play an important role for the magneto-conductance profile. Conductance resonances with perfect transmission from a certain input to one or several output terminals occur near the Dirac point energy when input and output(s) have gapless subbands with aligned spin polarization, for which we have derived a general criterion. These magnetotransport resonances depend crucially on the spin-momentum locking properties of the surface states and could be relevant for future quantum transport experiments as well as for 3D TI-based circuits for Majorana-based quantum information processing, as multi-terminal nanostructures form their basic building blocks (see Fig. 1 (d)). More details can be found in [3].

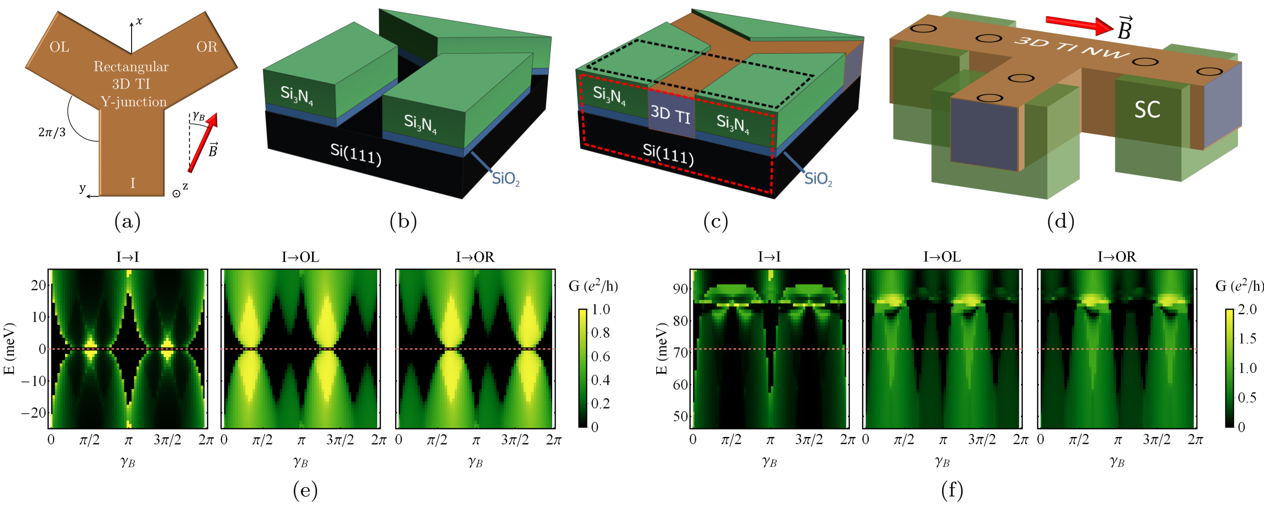

FIG. 1. (a) A 3D TI Y-junction with rectangular nanowire leads (top view). (b-c) Selective area growth of a 3D TI Y-junction. (b) A Si(111) substrate with a Si_3N_4/SiO_2 mask layer is pre-structured. (c) During MBE growth, the substrate temperature is adjusted such that the 3D TI only nucleates on the Si(111) surface. (d) A 3D TI T-junction with each leg containing a proximitized superconducting (SC) region. Pairs of Majorana bound states can appear in the regions along the length of the wire indicated by the black circles by tuning the relative superconducting phases and the external magnetic field appropriately. (e-f) The conductance between the different legs of a 3D TI nanowire Y-junction (see Fig. 1 (a)) is shown as a function of the angle γ_B of the magnetic field (with amplitude $|\mathbf{B}| = 2\Phi_0/\mathcal{A}$, $\Phi_0 = -h/e$ the magnetic quantum flux and $\mathcal{A}$ the cross section of the leads) and the energy level of the input leg. A (e) toy model (f) Bi_2Se_3 parameter set was considered, and the Dirac point energy of the corresponding 3D TI bulk system is indicated with a pink dashed line.

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Bulk Fermi arcs in heavy fermion systems

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We find that heavy fermion systems can have bulk "Fermi arcs", with the use of the non-Hermitian topological theory. In an interacting electron system, we can define the effective Hamiltonian $H_{\rm eff} \equiv H + \Sigma$, , where the microscopic many-body Hamiltonian is Hermitian, but the one-body quasiparticle Hamiltonian is non-Hermitian due to the finite quasiparticle lifetime. A possible mechanism of a Fermi arc has proposed in a Dirac material in two dimensions[1,2]. By introducing a topological theory of finite-lifetime quasiparticles, we can find that the low-energy dispersion of the Dirac material is reshaped and a topologically protected bulk Fermi arc appears. Finite quasiparticle lifetime is a generic property of quantum many body systems, resulting from either inelastic electron-electron/electron-phonon scattering at finite temperatures, or elastic electron-impurity scattering. The exceptional points of the non-Hermitian quasiparticle Hamiltonian matrix play a crucial role. With the use of the dynamical mean field theory (DMFT) calculation, we confirm our statement in Kondo insulators with a momentum-dependent hybridization in two-dimensions. We show that the concept of the exceptional points in the non-Hermitian quasiparticle Hamiltonian is one of powerful tools to predict new phenomena in strongly correlated electron systems.

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Nodeless superconductivity in type-II Dirac semimetal $PdTe_2$: low-temperature London penetration depth and symmetry analysis

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Superconducting gap structure was probed in type-II Dirac semimetal $PdTe_2$ by measuring the London penetration depth using tunnel diode resonator technique. At low temperatures, the data for two samples are well described by weak coupling exponential fit yielding $\lambda(T=0) = 230$ nm as the only fit parameter at a fixed $\Delta(0)/T_c = 1.76$, and the calculated superfluid density is consistent with a fully gapped superconducting state characterized by a single gap scale. Electrical resistivity measurements for in-plane and inter-plane current directions find very low and nearly temperature-independent normal- state anisotropy. The temperature dependence of resistivity is typical for conventional phonon scattering in metals. We compare these experimental results with expectations from a detailed theoretical symmetry analysis and reduce the number of possible superconducting pairing states in $PdTe_2$ to only three nodeless candidates: a regular, topologically trivial, s-wave pairing, and two distinct odd-parity triplet states that both can be topologically non-trivial depending on the microscopic interactions driving the superconducting instability.

The experimental work was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. The experimental research was performed at Ames Laboratory, which is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358. N.H.J. is supported by the Gordon and Betty Moore Foundations EPiQS Initiative (Grant No. GBMF4411). M.S.S. acknowledges support from the German National Academy of Sciences Leopoldina through grant LPDS 2016-12. P.P.O. acknowledges support from Iowa State University Startup Funds.

Band structure engineering in 3D topological insulators

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We will present our recent combined experimental and theoretical results on the band structure engineering in 3D topological insulator (3D TI) bilayers [1] and superlattices [2] grown by molecular beam epitaxy (MBE) on Si(111). These studies show how new topologies emerge in complex structures, as compared to the routine Fermi level control by alloying [3, 4]. Our results provide a starting point in search for novel topological phases.

MBE growth of Sb_2Te_3 and Bi_2Te_3 leads to the p-type and n-type material respectively, due to the low formation energy of charged vacancies and antisites. We have succeeded in growing high quality heterostructures of Sb_2Te_3 grown on Bi_2Te_3 as confirmed by atomic resolution transmission electron microscopy images. The heterostructures form a vertical p-n junction where the Fermi level position at the surface can be controlled by the thickness of the two layers, which has been confirmed by photoemission [1].

Bi-Te compounds can be grown at various stoichiometries, which on the atomic level are combinations of Bi_2Te_3 quintuple layers and Bi bilayers. The Bi_1Te_1 stoichiometry results from combining two Bi_2Te_3 quintuple layers with one Bi bilayer in the unit cell. In such superlattice new dual topological properties emerge. According to our theoretical predictions the material is simultaneously a topological crystalline insulator (TCI) and a weak topological insulator (WTI), and photoemission results demonstrate the existence of TCI crossings away from the Brillouin zone center [2]. This opens up the possibility of controlling the topological protection on different surfaces selectively by breaking respective (mirror or time-reversal) symmetries.

Encouraged by these results we propose future research directions, which include preparation of heterostructures based on ferromagnetic insulators, and search for 2D materials which exhibit non-trivial topologies. In particular, we are optimizing the EuO thin films as ferromagnetic insulator substrates which may enable realization of QAHE by deposition of monolayers of heavy metals. With high-resolution photoemission we are searching for band crossings in ferromagnets which locally exhibit non-zero Berry curvature, as these contribute to the intrinsic contribution to AHE, with one example being demonstration of spin-orbit gaps in Fe(001) thin film [5].

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Optical and magneto-optical studies of topological nodal semimetals

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Topological nodal semimetals (TNSMs) currently attract enormous interest. Theory predicts that the (magneto)-optical response of TNSMs is not only distinct from the response of "ordinary" semiconductors and metals, but also sensitive to the TNSM's band structure and band dimensionality. The square-root magnetic-field dependence of inter-Landau-level transitions is well known as a fingerprint of linear electronic bands [PRB **69**, 075104 (2004)]. The frequency dependence of the optical conductivity, $\sigma(\omega)$, as such, also provides important relevant information [PRL **108**, 046602 (2012); PRB **87**, 125425 (2013)]. For example, 3D linear electronic bands, crossing at a point node at the chemical potential, are supposed to manifest themselves in a linear-in-frequency optical conductivity, while in the case of 2D linear bands $\sigma(\omega)$ should be frequency independent.

In the real TNSMs, nodes are rarely located at the chemical potential. Thus, free-electron absorption is essential. Additionally, topologically trivial parabolic bands are often present in the vicinity of chemical potential. Both effects may mask the theory-predicted behavior of the interband $\sigma(\omega)$, as well as the $\sqrt{B}$-proportional features in the magneto-optical spectra.

We have studied a large number of TNSMs (TaAs family, half-Heusler compounds, ZrSiS at its relatives, etc.) by means of optics and magneto-optics [PRB **93**, 121202 (2016); PRB **95**, 155201 (2017); PRL **119**, 187401 (2017); arXiv:1803.09708; arXiv:1803.00840]. Some of the studied materials have been affected by the aforementioned effects quite substantially. In the others, the low-energy (magneto)-optical response, related to the nodes and linear bands, is clearly observed. In Fig.1, we present a short summary of our most bright results for three different TNSMs.
(**I**) In GdPtBi, the linear increase of $\sigma(\omega)$ strongly suggests 3D linear electronic bands crossing each other near the chemical potential. This picture is in contrast with the widely adopted band structure (touching parabolic bands) of GdPtBi, but in qualitative agreement with most recent band-structure calculations [PRL **119**, 136401 (2017)].
(**II**) In the nodal-line semimetal ZrSiS, the observed frequency-independent $\sigma(\omega)$ evidences a 2D character of the linear electronic bands: the presence of a nodal line effectively reduces the band dimensionality. The absolute value of the flat $\sigma(\omega)$ is related to the length of the nodal line in reciprocal space [PRL **119**, 147402 (2017)].
(**III**) In TaAs, the frequency of the magnetic-field-induced absorbtion mode follows a $\sqrt{B}$ behavior, evidencing that the transitions, responsible for this mode, are between the Landau levels in linear bands.
More discussion on our findings will be given in the course of the presentation.

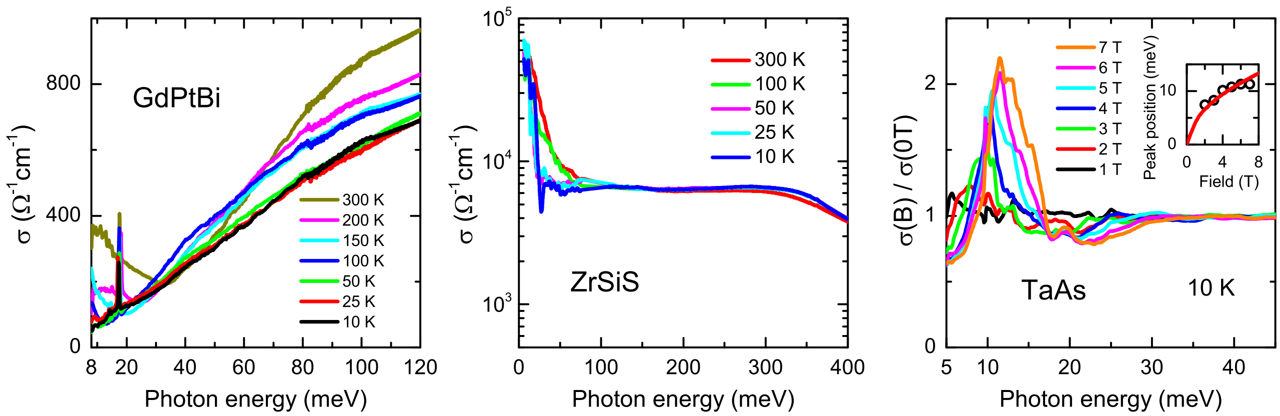

FIG. 1: Real part of the optical conductivity of GdPtBi and ZrSiS (left and centered panels, respectively) and normalized magneto-optical conductivity of TaAs (right panel). The inset shows the frequency position of the field-induced mode in TaAs. Note different scales on different panels.

Transport signatures of Majorana bound states in topological Josephson junctions

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In this talk, I will discuss a tunable Josephson junction in silicene where an electric field can switch between a 2π- and 4π-junction when two s-wave superconductors are placed on top of the silicene sheet. At a mass domain created by regions of different electric fields, either valley-chiral and spin-helical or valley-chiral and spin-degenerate edge states form accounting for a 4π- or a 2π Josephson effect, respectively. I also discuss possible experimental strategies to distinguish between a 2π- and 4π-junction. In a second part of the talk, I will discuss a novel Corbino geometry topological Josephson junction that hosts rotating Majorana bound states (MBS) in Josephson vortices. The current through an STM tip coupled to the junction shows clear signatures of the braiding of the MBS.

Crystallization of Levitons in the fractional quantum Hall regime

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The emergence of self-organized regular patterns in optical solitons has been recently subject of intense investigation, as they promise to be exceptionally useful in quantum communication [1]. In the framework of electron quantum optics, a train of Lorentzian voltage pulses emerges as the solid state counter-part of optical solitons, namely robust ballistically propagating wave-packets carrying an integer number q of electrons called Levitons [2,3]. Using a periodic train of Levitons, we investigate the charge density backscattered off a quantum point contact in the fractional quantum Hall regime, finding a self-organized and regular pattern of peaks and valleys[4]. We demonstrate that the predicted features manifest themselves as unexpected additional dips in the well-studied Hong-Ou-Mandel noise.

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Majorana Superconducting Qubits

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Topological superconductors hosting spatially well-separated Majorana bound states offer the possibility for realizing robust qubits protected from local environmental perturbations. Revealing new properties of Majorana bound states as well as establishing an experimentally feasible platform for Majorana-based quantum computing constitute two of the most urgent challenges in the field. In this talk, I will address these issues by discussing two setups of topological superconductors coupled to conventional superconductors:

(1) The first setup comprises a Coulomb-blockaded time-reversal invariant topological superconductor island with Majorana Kramers pairs placed in an s-wave superconductor Josephson junction. I will discuss a 2Pi Josephson effect which is mediated by the Majorana Kramers pairs and whose direction is controlled by the joint parity of all four Majorana bound states on the island, a "Parity-controlled 2Pi Josephson effect".

(2) The second setup constitutes a Majorana-based qubit in an all-superconducting circuit, a "Majorana Superconducting Qubit". I will demonstrate how universal quantum computation can be achieved in such a device and discuss advantages over conventional superconducting qubits.

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Discovery of new topological fourfold and sixfold Fermions and their Fermi arcs in a chiral crystal

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After the discovery of topological insulators, the search for new topological materials has led to the discovery of topological Dirac- and Weyl- semimetals, which host fourfold- and twofold-degenerate band crossings, respectively, and can be considered as the condensed matter realizations of free Dirac- and Weyl-Fermions that are known from particle physics. Recently, theoretical studies proposed the existence of Fermionic excitations in chiral crystals that go beyond Fermionic particles known from the Standard Model, namely threefold, sixfold and eightfold degenerate band crossings, which are referred to as “new Fermions” [1]. Interestingly, these higher order band crossings are located at high symmetry points and carry a topological charge (i.e. a Chern number) that is larger than the one in Weyl Fermions, and as a result, one can expect the existence of topological surface states on some surfaces, which form multiple Fermi arcs that connect the projections of higher order band crossings of opposite topological charge in momentum space. Detecting these Fermi arcs can therefore be considered as finding the fingerprint of the topological character of these new Fermions, which distinguishes them from the recently discovered topologically trivial triple points in MoP [2] and WC [3]. Most interestingly, if such new topological Fermions can be found in a chiral crystal, it may serve as a platform to realize exotic chiral transport phenomena - such as the circular photogalvanic effect [4] - which originate from the nontrivial Chern number of the new Fermions, and which cannot be observed in all previously discovered non-chiral Weyl-semimetals.

Here, we will present most recent results of our soft X-ray angle-resolved photoemission (ARPES) measurements of a chiral crystal, which shows clear signatures of new fourfold and sixfold Fermions, as well as results from VUV-ARPES experiments, which indicate the presence of Fermi arc surface states, thus confirming a nontrivial Chern number associated with these new Fermions.

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The Superconductivity of Topologically Protected Surface States

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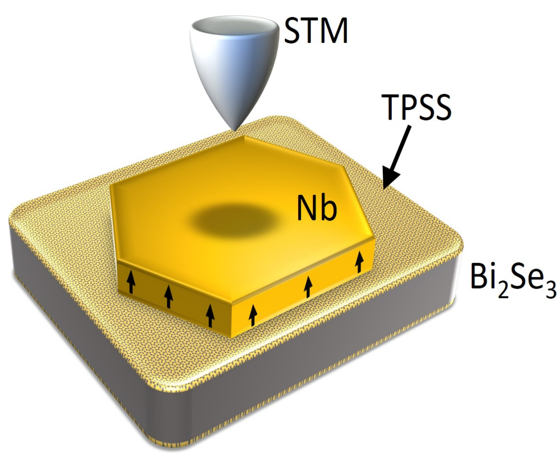
The superconducting proximity effect induced in materials in close contact with a superconductor is well known. Similarly the topologically protected surface states recently found on the surfaces of special crystals can leak into appropriate adjoining materials. We bring these two effects into proximity and study how superconductivity and topologically protected surface states interact with each other[1], a situation of interest in the search for Majorana bound states. We look at the scanning tunneling microscopy of a large topological insulator with superconducting islands deposited on the surface, and analyze theoretical models which capture the hybridization between the topological surface states and the superconducting states. The density of states of both the topological insulator and the superconductor turn out to exhibit interesting proximity effects and open up new possibilities for observing Majoranas.



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Surface magnetism and Dirac gap opening in antiferromagnetic Gd-doped topological insulator and its modification under synchrotron radiation photoexcitation

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In recent years, magnetically-doped topological insulators (TIs) have attracted enhanced interest due to possibility of effective realization Quantum Anomalous Hall effect (QAHE). The key challenge to realizing the QAHE is to simultaneously achieve low bulk carrier density and ferromagnetic ordering that assumes opening of the gap at the Dirac point (DP) due to the magnetic doping and localization of the gap at the Fermi level (FL) with formation of the chiral edge states inside the gap. However, magnetic transition metals act as not only magnetic dopants, but also as electric dopants, because they are usually divalent. This problem can be solved by the rare-earth metals doping of TIs instead of transition metals. Gd is trivalent and has an equal number of bonding electrons to Bi, therefore, no free carriers are introduced by the isoelectric substitution of Gd into TI. In the case, when no both any valence or conduction band (VB, CB) states are localized at the FL a significant contribution of the 2D surface Dirac-fermion-mediated magnetic coupling is expected. The electronic structure of Gd-doped TIs is characterized by antiferromagnetic ordering in the bulk. Therefore, study of such kind TIs may improve understanding of the surface magnetism in antiferromagnetic TIs and a coupling between the electronic structure and magnetic ordering in such systems. The current work is devoted to analysis of an origin of surface magnetic ordering in Gd-doped TI with stoichiometry $Bi_{1.0}Gd_{0.06}Sb_{0.85}Te_3$ characterized by localization of the Dirac gap near the FL developed above the Curie (Niele) temperature (with antiferromagnetic coupling in the bulk). Localization of the Dirac gap at the FL in this compound (without crossing FL by the CB and VB states) assumes a significant contribution of the 2D Dirac-fermion-mediated magnetic coupling in the surface magnetic ordering. For analysis a combination of ARPES, SQUID and XMCD methods was used. The changes the features of the topological surface and the VB structure by ARPES in the region of the gap at the DP arranged near the FL under photoexcitation by linear and circularly polarized synchrotron radiation (SR) were analyzed. SR of different chirality can rotate the magnetic moment that allows to manipulate by the Dirac gap value and the SR-induced out-of-plane and in-plane local magnetization. Role of the 2D surface Dirac-fermion-mediated magnetic coupling in the Dirac gap modification will be discussed.

Stability of Disordered Floquet Topological Phases

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In modern experiments, high-frequency periodic driving can be used to create new Floquet topological phases of matter. Taking into account the complex nature of finite-frequency disorder contribution to the Floquet Hamiltonian, one may wonder about the stability of these systems against static disorder. We leverage on modern free probability theory and ideas in random matrices to predict the fate of finite frequency Floquet topological phase in the presence of the disorder. We confirm, depending on disorder strength, the existence of gapped topological and gapless trivial phases, as well as a transition between them at a critical disorder strength. The method can be applied to a variety of Floquet models and shows a good agreement with numerical simulations.

Magnetization current and anomalous Hall effect for massive Dirac electrons

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Existing investigations of the anomalous Hall effect (*i.e.* a current flowing transverse to the electric field in the absence of an external magnetic field) are concerned with the transport current. However, for many applications one needs to know the total current, including its pure magnetization part. In this paper, we employ the two-dimensional massive Dirac equation to find the exact universal total current flowing along a potential step of arbitrary shape. For a spatially slowly varying potential we find the current density $\mathbf{j}(\mathbf{r})$ and the energy distribution of the current density $\mathbf{j}^{\varepsilon}(\mathbf{r})$. The latter turns out to be unexpectedly nonuniform, behaving like a δ-function at the border of a classically accessible area at energy ε. To demonstrate explicitly the difference between the magnetization and transport currents we consider the transverse shift of an electron ray in an electric field.

Topological Phase Transitions in Quantum Confined Topological Crystalline Insulator Heterostructures

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Topological crystalline insulators (TCI) based on the narrow gap lead-tin chalcogenide IV-VI semiconductors provide a unique platform for studying topological phase transitions due to their high sensitivity to strain, temperature and composition as well as external perturbations such as pressure and electric fields. In this work, we report on tuning topological phases by band gap egineering of quantum confined topological crystalline heterostructures and super-lattices grown by molecular beam epitaxy on different substrates in the (111) and (100) orientations [1,2]. Normal insulator $Pb_{1-y}Eu_ySe$ with wider band gap is used as barrier material onto which high mobility $Pb_{1-x}Sn_xSe$ QWs are deposited with thicknesses ranging from 3 to 40 nm and Sn contents x_{Sn} varying from 0 to 36%, spanning the whole range from the normal insulator to the inverted TCI side. The electronic band structure is investigated by angle resolved photoemission spectroscopy (ARPES) and theoretical tight binding calculations.

Our results reveal the formation of a series of very sharp QW states both in the conduction and valence band (see Fig. 1) with QW indices up to $i = 4$ and 8, respectively, exhibiting line widths as small as 10 meV. For thin QWs, the interactions between the top surface and bottom interface states of the QW layers opens an energy gap in the topological state due to hybridization, which characterized the penetration depth of surface and interface states. Surprisingly, this gap persists up to rather large QW thickness of 20 nm, which much exceeds the value observed for Bi-chalcogenide topological insulator thin film structures and it also depends on the surface orientation. The topological phase transition is studied as a function of temperature and composition, revealing that the decay of the surface and interface wave functions depends on the value of the inverted bulk energy gap and thus can be controlled both by the Sn content and the temperature. In the TCI state, the topological QW states exhibit not only a linear Dirac like energy momentum dispersion but also a strongly enhanced ARPES intensity due to the concentration of the topological wave functions at the QW surface. Overall, engineering of the topological quantum well states provides a novel tuning know for modification and control of modify topological properties for device applications.

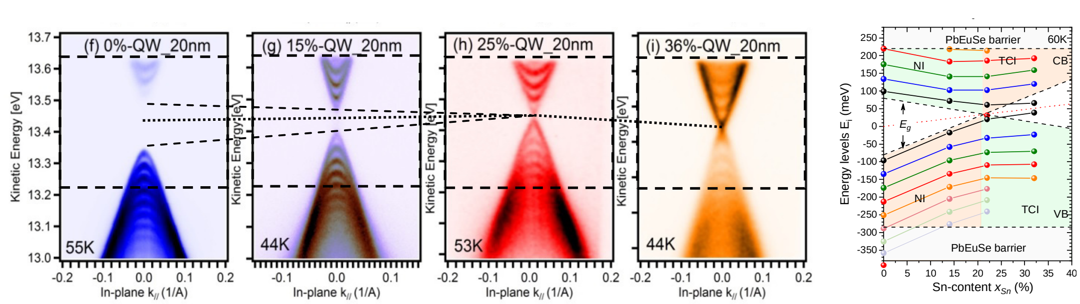

Figure 1: ARPES dispersions of PbSnSe/PbEuSe surface QWs with 20 nm QW thickness but different Sn content from 0 to 36% measured at around 50 K. The right hand side shows the derived energy levels as a function of Sn composition.

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Ultrafast carrier dynamics and transient population inversion of the topological insulators $(Sb,Bi)_2Te_3$

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Dirac materials possess Dirac fermions characterized by the zero-gap and conical band dispersions. Dirac fermions are realized in graphitic materials, on surface of topological insulators (TIs), and in three-dimensional Dirac semimetals. Dirac materials have the potential to revolutionize lasers [1]: If a population inversion can be maintained across the Dirac point of the conical band structure, induced emission can occur for whatever color. Wide-band mode locking is already demonstrated in a variety of Dirac materials [2], indicating that the optical filling of the upper Dirac cone is substantial when the optical pumping is intense enough. The surface of TIs may be used as an optical gain medium for broad-band lasing if the duration of an inverted population in the topological surface states (TSSs) can be elongated.

Time- and angle-resolved photoemission spectroscopy (TARPES) is a pump-and-probe method, and can visualize the electron distributions after the optical pump in a time-, energy-, and momentum-resolved manner. Being a surface sensitive method, TARPES is the suited method to verify the population inversions occurring on TIs. The first evidence for the population inversion in the TSS was found in a naturally hole-doped (p-type) TI, Sb_2Te_3 [3]. However, the duration of the inversion was ∼3 ps at most. Even though the ∼3-ps duration is longer than the non-thermal and possibly inverted distributions reported for graphitic materials [4], further elongation would be the requisite. In addition, from the application point of view, the demonstration is better done at room temperature, where thermally-activated electrons also exist and may affect the duration.

Here, we investigate the carrier dynamics of a p-type TI $(Sb_{1-x}Bi_x)_2Te_3$ by using TARPES. Our main focus is in the investigation into how the dynamics is affected by the thermally-excited carriers. We show that the duration of the nonequilibrated state is prolonged at elevated temperatures, where the thermally-excited electrons coexist and partially fill up to the Dirac point. Furthermore, the duration of the population inversion across the Dirac point is also prolonged from >7 ps at 8 K to >10 ps at 300 K in $x = 0.27$. We attribute the elongation to the thermally enhanced blocking near the Dirac point at 300 K. Our finding shows the ability to control the degree of population inversion and paves a way to the realization of broad-band lasing and other optoelectronic functions using TIs.

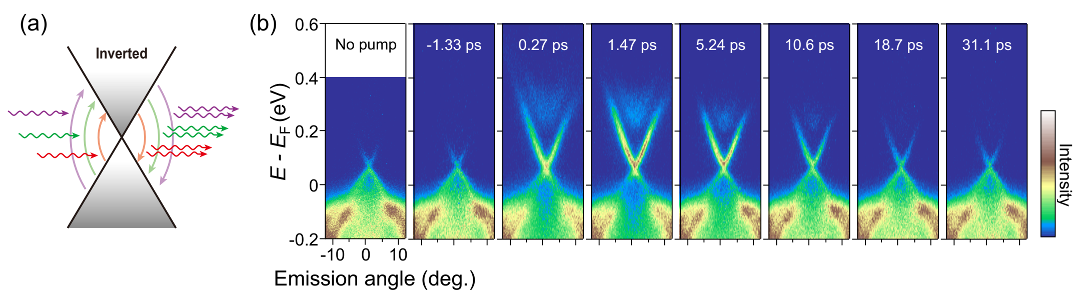

FIG. 1: (a) Schematic of population inversion and broad-band lasing in Dirac material. (b) Photo-excited carrier dynamics in the $(Sb_{0.73}Bi_{0.27})_2Te_3$ crystal. TARPES images recorded at various pump-probe delay times at 300 K.

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Exotic phenomena observed by transport measurements in a topological insulator

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Topological insulators are promising candidates for spintronic applications, as they have protected surface state robust against disorder, their symmetry forbid back-scattering and have spin-current. Recently, it has been reported that there is a systematic discrepancy between optical measurements (ARPES) and transport measurements (through quantum oscillations). The origin of this difference is not well understood and further investigations are needed.

We present transport measurements of the bulk insulating topological insulator $TlBiSe_2$. Photo-induced phenomena and exotic current-voltage (IV) characteristics have been observed. By illuminating the sample, different states seems to emerge, like the existence of a hidden metallic state. Simultaneously, IV curves present a switching behaviour with hysteresis. These effects can be understood by introducing localized states on the surface. A unifying picture that would also fit the results reported in the literature is attempted.

Magnetoresistance induced by GeTe/Sb_2Te_3 topological chalcogenide superlattices

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A chalcogenide alloy, Ge-Sb-Te (GST) is the most important as a recording material not only for rewritable digital versatile disc (DVD) but also for electric non-volatile memory (NVM), which was commercialized by Intel and Micron Technology in 2017.[1] The NVM was named "*Optane*", in which a GST alloy was used as a phase-change memory (PCM) film. The switching mechanism of *Optane* is very simple, and relies on the phase transition of the GST alloy in between the amorphous ($RESET$) and crystalline (SET) states, which are performed using a high or low electric current injection with a specific time duration. A typical switching time is 100 ns or less, and the required current for $RESET$ is about a few hundreds μA.

Although *Optane* is the most successful product for NVM at the moment, a further advanced PCM called interfacial phase-change memory ($iPCM$) has been developed since 2008.[2] $iPCM$ does not use the amorphous-crystal phase transition for memory switching despite using GST alloy. Instead, the memory film is consisted of a multilayer or superlattice, in which crystalline sublayers of GeTe and Sb_2Te_3 are alternatively stacked with a certain film thickness determined by $ab-initio$ computer simulations. As known well, Sb_2Te_3 is a topological insulator TI, while GeTe is a band-gap normal insulator NI. Therefore, the perfect superlattice is consisted of a repetition of $(TI/NI)_n$, where n is an integer.[3] $iPCM$ was not invented to emerge TI characteristics at the beginning, but to reduce the switching energy in the transition from SET to $RESET$ in PCM by suppressing the entropy loss due to the three-dimensional Ge atomic motions.[4] Soon later, we noticed that the $iPCM$ structures may provide a platform to understand the properties of TIs. Since 2011, we first discovered that $iPCM$ has a large magnetoresistance (MR) effect at room temperature under 0.1 T magnetic field while a *SET-RESET* cycle test was carried out using the memory device.[5] Later, we noticed that the MR is never presented only by an external magnetic field, but is accompanied by injection of current pulses that penetrate the superlattice from the top to the bottom(or vise versa).[6] In addition, it was found that the MR effect is further enhanced after annealing at 470K for 2 or 4 hours followed by cooling under a magnetic field. We reported in ref.[6] that the large MR effect only occurs at the certain GeTe thickness of 0.4 nm and 0.8 nm, corresponded to a GeTe monolayer and the bilayer. It is noted that GeTe may exist a 2D atomic sheet with an electric dipole. Fig. 1 shows the device structure and the MR effect when an external magnetic field was scanned in between -0.5 T and +0.5 T.

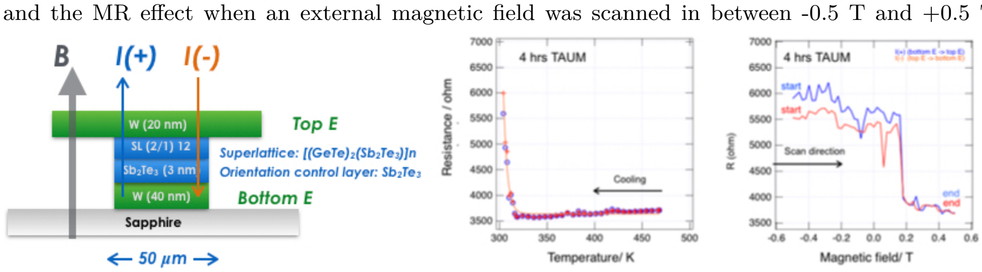

Fig. 1(left) cross-section of the device, (center) resistance change when the device is cooled from 470K to room temperature under -0.5 T magnetic field, and (right) magnetoresistance when the magnetic field is scanned from -0.5 T to +0.5 T. In the reverse scan, the resistance is almost constant with the value at +0.5 T over the scanning range (not shown).

We report the unique characteristics of $(TI/NI)_n$ superlattices in the workshop.

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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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