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14. ABSTRACT

This document, a record of the workshop "New Trends in Topological Insulators", lists abstracts from 33 papers and 34 posters present at the conference. Topics cover various aspects of topological insulators including different physical compositions, surface and interface states, electromagnetic responses, Majorana fermions, and many more.

15. SUBJECT TERMS

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WORKSHOP

New Trends in Topological Insulators

Sant Feliu de Guíxols
Barcelona - Spain
3-6 June 2013

ABSTRACTS BOOK

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POSTERS

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

HgTe as a topological insulator

Laurens W. Molenkamp*

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Abstract

HgTe is a zincblende-type semiconductor with an inverted band structure. While the bulk material is a semimetal, lowering the crystalline symmetry opens up a gap, turning the compound into a topological insulator.
The most straightforward way to do so is by growing a quantum well with (Hg,Cd)Te barriers. Such structures exhibit the quantum spin Hall effect, where a pair of spin polarized helical edge channels develops when the bulk of the material is insulating.
Our transport data[1-3] provide very direct evidence for the existence of this third quantum Hall effect, which now is seen as the prime manifestation of a 2-dimensional topological insulator.
To turn the material into a 3-dimensional topological insulator, we utilize growth induced strain in relatively thick (ca. 100 nm) HgTe epitaxial layers. The high electronic quality of such layers allows a direct observation of the quantum Hall effect of the 2-dimensional topological surface states[4]. Moreover, on contacting these structures with Nb electrodes, a supercurrent is induced in the surface states.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Mercury Telluride, a topological insulator with a helical spin texture

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Institut Néel et Université Joseph Fourier Grenoble

Abstract

Topological insulators describe materials that are conducting on the surface but insulating in the bulk. Such unique property has its origin in the non-trivial topological structure of the set of wave functions $\{\psi_k(r)\}$ when the momentum k spans the Brillouin zone. Usual insulators have positive gaps while topological insulators are found in material with inverted band structures (negative gaps).
Mercury Telluride is a semi-metal with an inverted band structure. It can be turned into a topological insulator by applying a bi-axial stress, as the one occurring in epitaxial growth from a substrate with slightly different lattice constants.
We have measured surface and bulk band structures of Mercury Telluride by Angle Resolved Photo-Emission Spectroscopy (ARPES), on the CASIOPEE line at Soleil Synchrotron. We find the dispersion of surface states form a Dirac cone, with the top half lying inside the stress-gap and into the conducting band. The bottom half lies within the hole-band. The Dirac point sits precisely at the top of the hole-band (within the experimental accuracy). In the experiments, the surface state dispersion stays linear between the Γ and the X points, well beyond the region where topological protection is expected to be effective.
We have also measured the circular dichroism of the photo-emitted electron intensity with respect to left-right polarization of incident photons. We find a dichroism coming from the surface and the bulk hole bands. While a dichroism of the surface states has been observed in other topological insulator, the strong dichroism signal coming from the bulk band is more surprising and shows that the bulk bands are spin-polarized.
The implication for transport experiments and spintronic devices will conclude the talk.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

A novel family of chiral-based topological insulators: Elemental tellurium under strain

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Abstract

The heavier group-VI elements selenium and tellurium are ubiquitous in most of the recently discovered binary or ternary TIs and exhibit a wide variety of interesting properties under pressure. They undergo complex structural changes, exhibit semiconductor-to-metal transitions, have unusual melting curves, and some of their high-pressure phases are superconducting at low temperatures. At ambient conditions, tellurium has a trigonal crystal structure (Te-I), consisting of weakly interacting infinite helical chains, arranged in a hexagonal array, which spiral around axes parallel to c. Each atom forms strong covalent-like intra-chain bonds with its two nearest neighbors (NN) and weak van der Waals-like inter-chain bonds with its four next NN. This unique feature is reflected in liquid-state studies of Te which showed that the chain structure is retained above the melting temperature.

Employing ab initio electronic structure calculations we predict [1], that trigonal tellurium consisting of weakly interacting helical chains, undergoes a trivial insulator to strong topological insulator (metal) transition under shear (hydrostatic or uniaxial) strain. In most reported TIs to date, the band inversion and the gap closing occur near the time-reversal invariant momenta (TRIM), where the frontier valence band (VB) and conduction band (CB) are doubly degenerate, as required by Kramer's theorem. In sharp contrast, the minimum band gap in Te-I occurs at a non-TRIM, where the two frontier VBs are non-degenerate while the doubly degenerate CB is protected by the three-fold screw symmetry of the helices. Thus, the transition to a TI state can be induced only by shear strain which breaks the three-fold symmetry and lifts the two-fold degeneracy of the CB state. We demonstrate the transition by examining the strain evolution of the band structure, of the topological Z2 invariant [2], and the concomitant band inversion. The underlying mechanism is the depopulation of the lone-pair orbitals, associated with the valence band, via proper strain engineering. Thus, Te becomes the prototype of a novel family of chiral-based 3D TIs with important implications in spintronics, magneto-optics and thermo-electrics, including chirality-induced spin selectivity, where spin-polarized electrons have different tunneling properties in right- and left-handed helices depending on the electron spin polarization relative to the direction of sense advance of the helix.

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This work is supported by NSF under Grant No DMR-1205734.

Figure

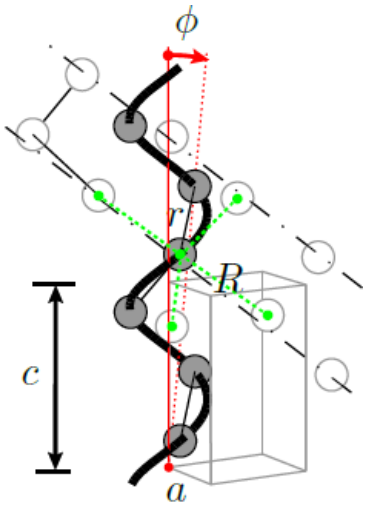

Figure Caption. 3D and top views of trigonal Te-I consisting of right-handed helical chains arranged on a hexagonal lattice. Each atom has two intra-chain NN and four inter-chain next NN with bond lengths r and R, respectively. The dot-dashed lines show Kreb mesomeric chains. The shear strain tilts the axes of all chains with respect to the c axis by an angle -

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Topological Surface States : Discovery and Recent Results

M.Z.Hasan

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http://www.princeton.edu/physics/people/display_person.xml?netid=mzhasan&display=faculty

Abstract

Topological Insulators are a new phase of electronic matter which realizes a non-quantum-Hall-like topological state in the bulk matter and unlike the quantum Hall liquids can be turned into superconductors at the bulk and/or at the interface.

First part of this talk highlights experimental demonstration of Z2 topological order via bulk-boundary correspondence as it its original definition (Kane-Mele). Experimental results include demonstration of the fundamental properties of topological insulators such as spin-momentum locking, non-trivial Berry's phases, mirror Chern number, absence of backscattering, protection by time-reversal and other discrete symmetries and their persistence up to the room temperature (at the level of M.Z. Hasan and C.L. Kane, Rev. of Mod. Phys., 82, 3045 (2010)).

I will then present (exciting) recent results demonstrating broken symmetry phases such as superconductivity and magnetism in artificial hetero interfaces as well as outline the emerging experimental research frontiers of the field of topological insulators as a whole.

Time permitting, I will also present experimental results on a new class of topological insulators beyond the Kane-Mele Z2 theory.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Electronic structure of complex topological insulators and Rashba-type systems

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Abstract

Spin-orbit interaction underlies many bulk and surface phenomena with intriguing potential applications. It plays especially important role in the surface electronic structure leading to massless states on the surface of many narrow gap semiconductors (topological insulators) [1-7] and spin-split surface states on metals, semiconductors, and overlayers (Rashba-type systems) [8-10]. Here we present and discuss recent results for complex topological insulators and new Rashba-systems. Magnetic impurities [11] and magnetic proximity [12] effects on electronic structure of these materials are also discussed in detail.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

A sudden collapse in the transport lifetime across the topological phase transition in (Bi1-xInx)2Se3

Liang Wu[a,*], R. Valdes Aguilar [a], M. Brahlek [b] , A.V. Stier [a], Y. Lubashvsky, [a] C.M. Morris [a], L.S. Bilbro [a], N. Bansal [b], S.Oh [b], N.P. Armitage [a]

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Abstract

Topological insulators (TIs) are newly discovered states of matter with robust metallic surface states protected by the topological properties of the bulk wavefunctions[1,2]. Of particular interest is the quantum phase transition (QPT) between a TI to a conventional insulator. Such a transition between different topological classes can only occur when the bulk band gap closes[1,2]. In this work[3], we have utilized time-domain terahertz spectroscopy (TDTS) to investigate the low frequency conductivity in $(Bi_{1-x}In_x)_2Se_3$ as we tune through this transition by indium substitution. Above certain substitution levels we observe a sudden collapse in the transport lifetime that indicates the destruction of the topological phase. We associate this effect with the threshold where the states from opposite surfaces hybridize. The substitution level of the threshold is thickness dependent, but we find that it asymptotically approaches the bulk limit x~ 0.06 where a maximum in the mid-infrared absorption is exhibited. This absorption can be identified with the bulk band gap closing and change in topological class. Our work shows the fundamental role that finite size effects play in this transition though the `bulk-boundary correspondence' of topological systems.

References

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Acknowledgements

This work was supported by DOE grant for The Institute of Quantum Matter at JHU DE-FG02-08ER46544 and by the Gordon and Betty Moore Foundation. The work at Rutgers was supported by IAMDN of Rutgers University, NSF DMR-0845464 and ONR N000140910749/N000141210456.

Figure 1

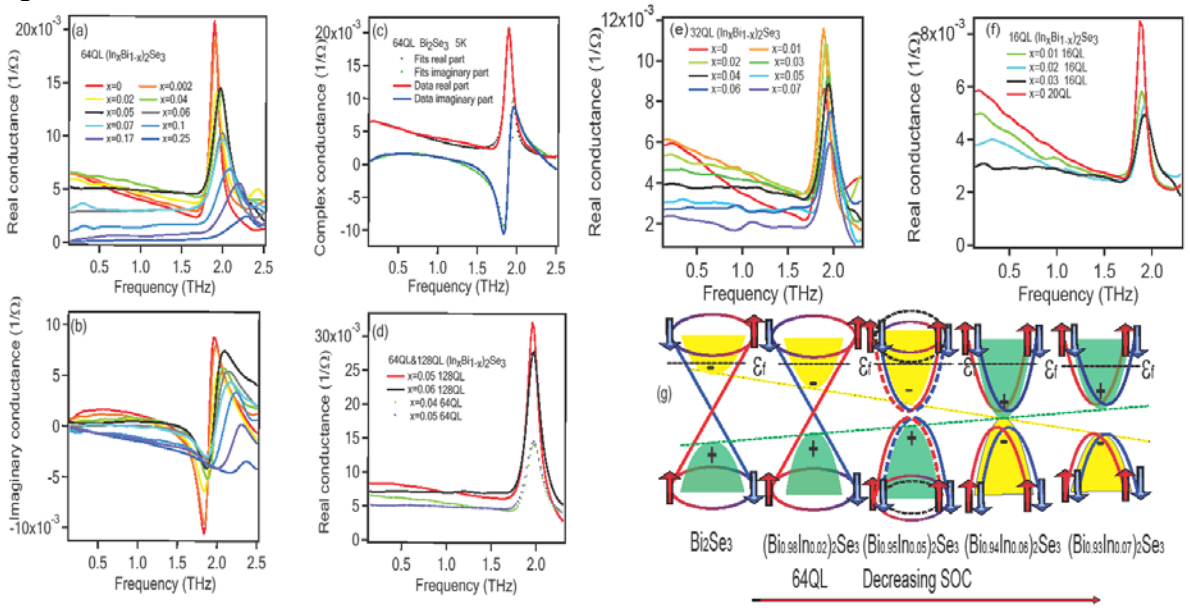

Figure Caption: (a) Real and (b) Imaginary parts of the THz range sheet conductance for different indium concentration levels (Bi1-xInx)2Se3 of 64QL films at 5K. QL means quintuple layer and equals 9.4 nm. A sudden broadening of the Drude peak is observed at x=0.05, as shown by the black curve. (c) Experimental data with fits for 64QL pure Bi2Se3 at 5K (d) Real parts of the THz range sheet conductance for 128QL (Bi1-xInx)2Se3 with selective In concentration at 5K. 64QL samples are included for comparison. From raw data, x=0.05 128QL sample has almost same slope (and therefore scattering rate) with x=0.04 64QL sample, while x=0.06 128QL and x=0.05 64QL samples shows the same flattening behavior of the Drude peak. (e), (f) Real parts of the THz range sheet conductance for 32QL and 16QL (Bi1-xInx)2Se3 at 5K respectively. A sudden collapse in transport time occurs at x=0.04 for the 32QL sample and x=0.03 for the 16QL sample, as also indicated by black curves. (g) A cartoon demonstration for bulk band inversion for 64QL series. With increasing In concentration, bulk band gap decreases, closes at x=0.06 and reopen afterwards. Inversion of valence (conduction) band parity is indicated by the solid yellow-green color and the plus-minus sign. At $x=0.05$ for the 64 QL sample, the TSSs hybridize and open a small gap. Solid and dashed curves stands for gapped Dirac cone from top and bottom surfaces respectively. Above x=0.06, trivial surface states may exist. Spin-up and spin-down branches in the non-TI regime are shifted just for clarity.

Figure 2

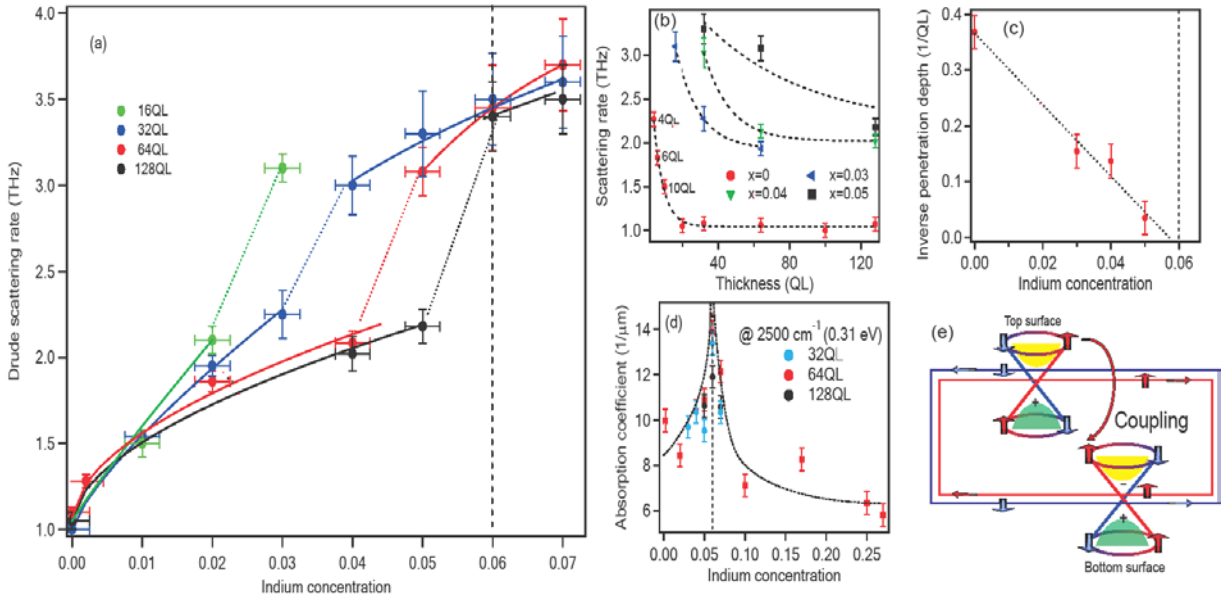

Figure Caption: (a) Scattering rate of Drude term from Drude-Lorentz fits as a function of indium substitution. Solid lines are guides to the eye. Jump in transport occurs at x=0.03, x=0.04, x=0.05 and x=0.06 for 16QL, 32QL, 64QL and 128QL series, respectively, as indicated by the dashed lines. The vertical black dashed line indicates where bulk band gap closes and band inverts. (b) Scattering rate as a function of thickness at different In concentrations. The dashed lines are fits 1/□= (a+b exp{-d/2□}) to extract 1□□ □ is TSS penetration depth and d is the film thickness in QLs. The 64 QL x=0.03 point is an interpolation from Fig. 1(a). (c) Inverse penetration depth 1/□ as a function of thickness. Dashed line is linear fit. Vertical dashed line indicates the topological phase transition. (d) Room temperature mid-infrared absorption coefficient at 0.31 eV (2500 cm^{-1} as a function of indium concentration for 32QL, 64QL and 128QL series, which all show the absorption peak at x=0.06. Dashed lines are guides to eye. (e) A cartoon picture that explains the jump in scattering rate: TSSs on top and bottom surface with opposite helicity become coupled and, therefore, open a new channel for scattering as states with the same spin and opposite momentum near the Fermi

level can scatter into each other. Blue and red lines demonstrate the spin-momentum locking mechanism. Up(red) and down(blue) spins move in the opposite directions.

Figure 3

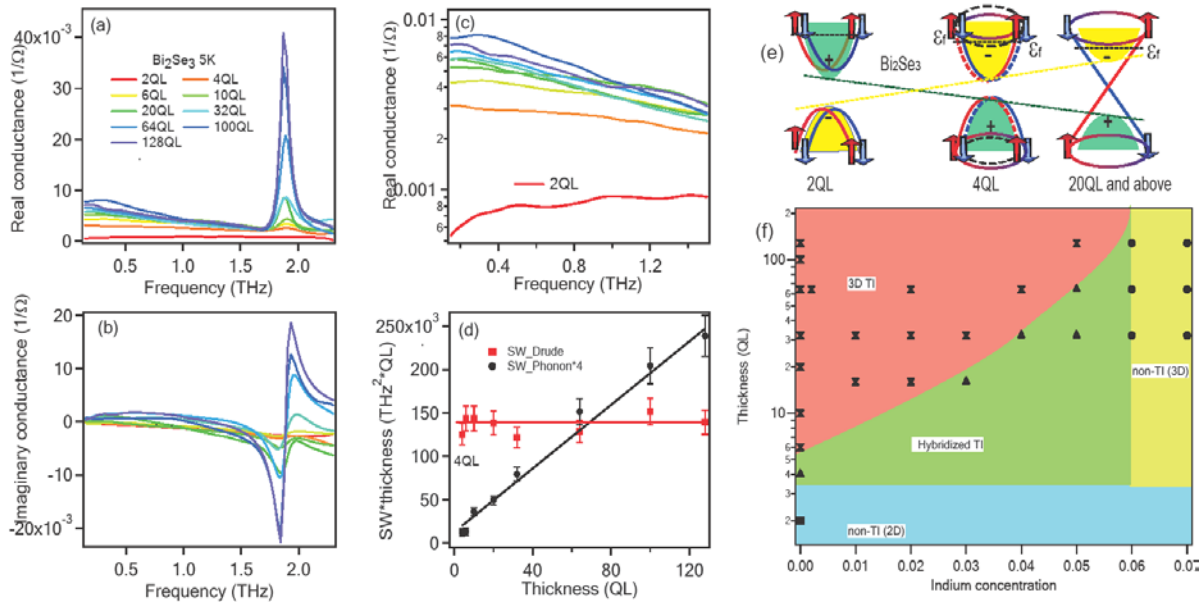

Figure Caption: (a) Real sheet conductance of pure Bi2Se3 films with different thickness at 5K. (b) Imaginary sheet conductance of Bi2Se3 films with different thicknesses at 5K. (c)The same data in panel (a) but on a log-linear scale to highlight low frequency conductance. (d) 2D Drude spectral weight (SW) ($\square_{pD}^2 d$) and 2D phonon spectral weight ($4\square_{ph}^2 d$) as function of film thickness. Solid lines are guides to the eye. (e) A cartoon picture shows how TSS hybridization occurs when film thickness is reduced. 4QL and 2QL films may be topologically non-trivial and trivial respectively as theoretically proposed. Spin-up and spin-down branches in the non-TI regime are shifted just for clarity. (f) A phase diagram constructed to distinguish different phases. Solid markers with different shapes correspond to experimental data in different regimes. The boundary between TI and the hybridized regime is set by the length scales determined by the fits in Fig.2(b).

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Dirac Equation in Topological Insulators and Superconductors

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Abstract

Topological insulators are insulating in the bulk, but process metallic states around its boundary owing to the topological origin of the band structure. The metallic edge or surface states are immune to weak disorder or impurities, and robust against the deformation of the system geometry. In this talk, I present a unified description of topological insulators and superconductors from one to three dimensions based on the modified Dirac equation. A series of solutions of the bound states near the boundary are derived, and the existing conditions of these solutions are described. Topological invariants and their applications to a variety of systems from one-dimensional polyacetylene, to two-dimensional quantum spin Hall effect and p-wave superconductors, and three-dimensional topological insulators and superconductors or superfluids are introduced. I shall introduce the bound states by the topological impurities and Majorana fermions in topological superconductors.

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Acknowledgements.

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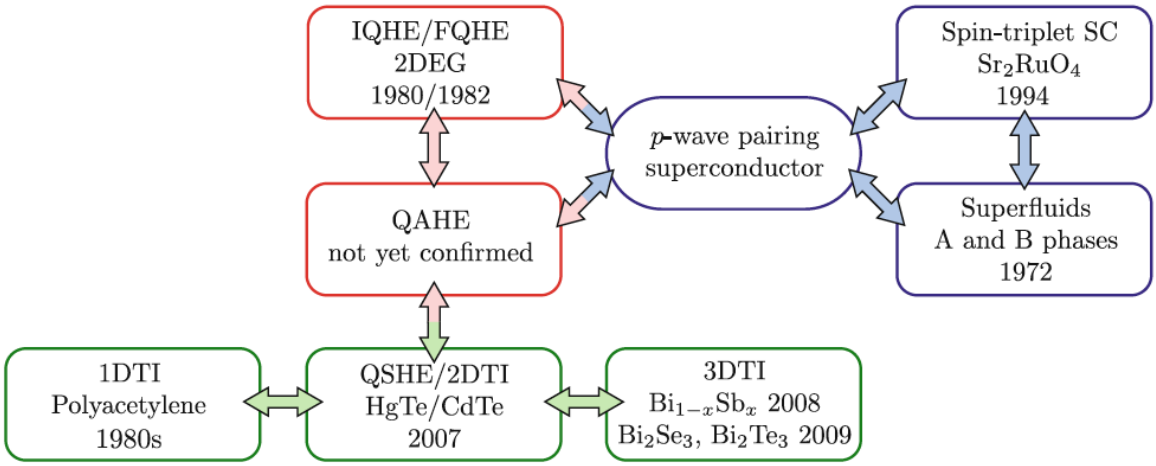
Figure

Figure Caption. Family tree of topological insulators and superconductors. The materials are followed by the year of discovery. Edge states in Sr_2RuO_4 need to be confirmed further. (adopted from Ref.[1])



Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Surface and Interface states of topological insulators

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Abstract

The surface states of three-dimensional topological insulators typically form Dirac cones, as has been shown experimentally in Bi_2Se_3 and Bi_2Te_3. The Dirac cones have well-defined chirality, which have two possibilities shown in Fig. (i) and (ii). This chirality corresponds to the sign of the velocity.

Topological insulators are characterized by the Z_2 topological number. Therefore, if two different topological insulators are attached together, the interface states between them usually become gapped because 1+1=0 (mod 2). In our presentation, we consider an interface between two topological insulators with opposite chiralities, and we show that in the presence of the mirror symmetry, the interface states become gapless. This comes from the mirror Chern number, defined in the cases with mirror symmetry. The topological insulators with opposite chiralities correspond to the mirror Chern numbers +1 and -1, and therefore the interface between them has +1-(-1)=2 Kramers pairs of interface states on the mirror plane. The overall interface states becomes a collection of Dirac cones, depending on other crystallographic symmetries (Fig.(iii)). We note that these interface states are protected by mirror symmetry and therefore are similar to the surface states of topological crystalline insulators [3]. We also demonstrate existence of gapless interface states using the Fu-Kane-Mele tight-binding model on the diamond lattice, and we show that with particle-hole symmetry the gap of the interface states closes along a loop, rather than at some Dirac points [2].

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Acknowledgements.

This work is supported by TIES, Tokyo Institute of Technology, and by the Asahi Glass Foundation.

Figure

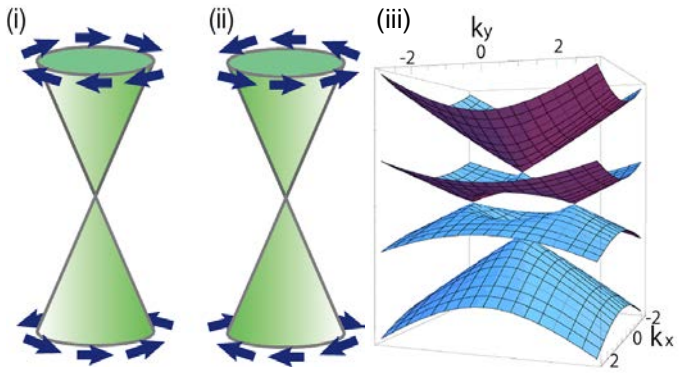

Figure Caption. Schematics of the surface Dirac cone with (i) positive chirality (velocity) and (ii) negative chirality (velocity). (iii) shows an example of band structure for the interface between two topological insulators with opposite velocities.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Edge states of 2D topological insulators explored by density-functional theory

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Abstract

The recent excitement about two-dimensional (2D) topological insulators (TIs) stems from the transport properties of their protected edge-states that provide a fascinating playground for basic and applied research. In practice, a 2D TI has to be supported by substrates that offer the possibility to tune materials properties, e.g. influence the structure by epitaxial constraints, enhance spin-orbit coupling effects by proximity effects or induce magnetic fields. All these effects can lead to a change of the topological invariants of the 2D TI, allowing for new properties. We will discuss these effects on the example of ultrathin Bi and Sb films, both freestanding [1] and supported [2] and in the presence of an exchange field [3]. Finally, the effect of edge reconstruction on the number of conductive channels of a Bi or Sb(111) bilayer ribbon is discussed. We show results of density-functional theory calculations together with experimental evidence, where available.

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Acknowledgements.

The work presented was carried out in collaboration with G. Bihlmayer, H. Zhang, F. Freimuth, I. Aguilera, C. Friedrich, H.-J. Kim, J.-H. Cho, and Y. Mokrousov. We acknowledge support by the Helmholtz Virtual Institute for Topological Insulators (VITI).

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Tuning the many body ground state of a system of Dirac quasiparticles

Pablo Jarillo

Abstract

In this talk I will present our recent experiments on quantum transport in graphene/hBN heterostructures in the quantum Hall regime, where we realize a quantized spin Hall effect in the absence of time reversal symmetry. This effect manifests itself as a conducting state due to helical counterpropagating edge states with conductance near 2 e^2/h, while the bulk remains insulating.

Workshop on NEW TRENDS in TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Engineering topological boundary states in topological insulators

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Abstract

In my talk I will cover our recent theoretical investigations directed towards developing new approaches for controlling topologically protected boundary states in topological insulators. In particular, I will focus on the dependence of electronic properties of topological states on the crystallographic orientation of the boundary.

In the first part of my talk I will consider the dependence of band dispersion of the quantum spin Hall effect (QSHE) edge states in the Kane-Mele model [1] on crystallographic orientation of the edges. It will be demonstrated that in this model system the Fermi velocities of the QSHE edge-state bands increase monotonically when the edge orientation changes from zigzag via chiral to armchair [2]. A simple analytical model explains the numerical results. I will then introduce a method for enhancing spin-orbit interactions in graphene nanostructures by means of covalent functionalization of the edges with functional groups containing heavy elements [3]. Proof-of-concept first-principles calculations show that very strong spin-orbit coupling can be induced in realistic models of narrow graphene nanoribbons with tellurium-terminated edges. We demonstrate that electronic bands with strong Rashba splitting as well as the quantum spin Hall state spanning broad energy ranges can be realized in such systems.

In the second part of my talk I will cover our recent results on high-index surfaces of bismuth chalcogenide topological insulators Bi_2Se_3 and Bi_2Te_3. The vast majority of research efforts have focused on the low-energy (111) surfaces which correspond to weak planes in the layered crystal structures. However, low-dimensional nanostructures such as nanowires and nanoparticles [4] will inevitably involve high-index facets. We perform a systematic ab initio investigation of the high-index surfaces of bismuth chalcogenides characterized by different crystallographic orientations as well as surface reconstructions and stoichiometries [5]. Several stable surfaces are shown to exist under varying thermodynamic equilibrium conditions. Surface orientation and stoichiometry are found to dramatically affect band dispersion and spin polarization of the topological surface-state charge carriers.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Title Topologically protected quantum transport in locally exfoliated bismuth at room temperature

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Abstract

We report conductance experiments in Bismuth nanocontancts created by repeated tip-surface indentation using a scanning tunneling microscope at temperatures of 4 K and 300 K [1]. We find a remarkable fact during the breaking process of the nanocontacts at room temperature: Robust long plateaus at the quantum of conductance G0 = $2e^2/h$ occasionally appear as a function of the elongation (see Fig. 1). The observation of shorter conductance steps below G0 before the final breaking of the nanocontacts at both temperatures indicates that these plateaus cannot be attributed to a single atom. We propose that these long plateaus are the result of the local exfoliation of a single Bi(111) bilayer (see Fig. 2) which has been predicted to be a quantum spin Hall insulator. Transport calculations confirm that Bi(111) bilayer flakes, despite of hosting three helical pairs, conduct as if a single pair existed when any type of imperfections are considered.

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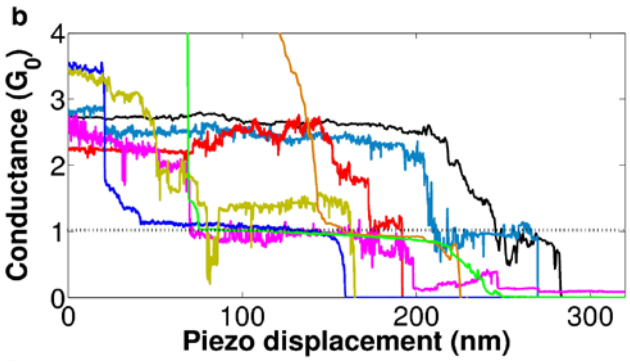
Figures



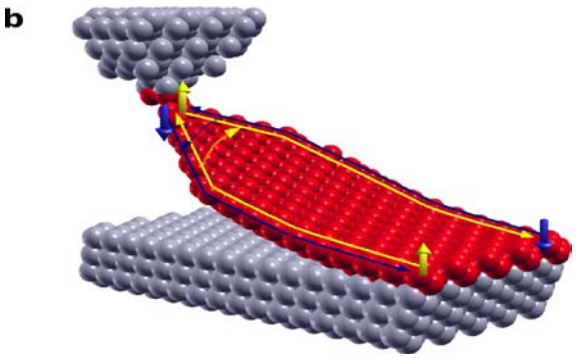


Figure Caption 1. Conductance traces at room temperature

Figure Caption 2. Proposed exfoliation mechanism

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Quasi-ballistic transport of Dirac fermions in a Bi_2Se_3 nanowire

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Abstract

Quantum coherent transport of Dirac fermions in a mesoscopic nanowire of the 3D topological insulator Bi_2Se_3 is studied in the weak-disorder limit. Nanostructures of Bi_2Se_3 were prepared by Chemical Vapor Deposition (CVD) without any catalyst. At very low temperatures, many harmonics are evidenced in the Fourier transform of Aharonov-Bohm oscillations, revealing the long phase coherence length ($L_\square$) of surface states. The strong Aharonov-Bohm contribution, which only results from surface Dirac fermions, superimposes on universal conductance fluctuations (UCF). Using a 3D-vector magnetic field, we reveal a dimensionality effect which is the signature of the quasi-1D nature of quantum coherent transport, showing that $L_\square$ is longer than the transverse dimension of the nanowire over the broad temperature range studied.

Remarkably, from their exponential temperature dependence, we infer an unusual $1/T$ power law for the phase coherence length $L_\square(T)$. This typical temperature dependence indicates the weak coupling of the fermions to the dynamics of their environment. Another important outcome is the evidence of the quasi-ballistic transport regime of spin-chiral Dirac fermions over the perimeter of the Bi_2Se_3 nanowire (~ 240 nm), a much longer length scale compared to the inter-defect distance (~ 5 nm for a residual doping of 10^{19} cm^{-3}). This is a signature of the weakening of the transport scattering time for spin-chiral fermions.

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Figure

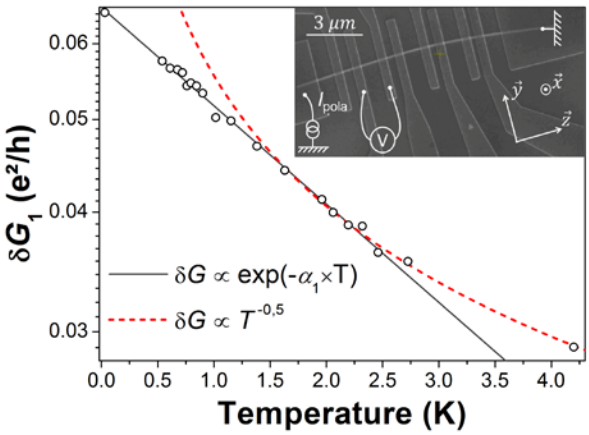

Figure Caption. Temperature dependence of the integrated fundamental harmonic, showing a clear exponential decay from 30 mK up to about 2.5 K. The high-temperature 1/sqrt(T) regime is shown as a dotted line. The inset show a SEM picture of the nanowire, with a rectangular cross-section (w = 90 nm, d = 50 nm) and a length of about 18 µm.

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Topological insulators and their implications for electronic order

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Abstract

Much of condensed matter physics is concerned with understanding how different kinds of order emerge from interactions between a large number of simple constituents. In ordered phases such as crystals, magnets, and superfluids, the order is understood through symmetry breaking. A major discovery of the 1980s was that electrons confined to two dimensions and in a strong magnetic field exhibit a completely different, "topological" order in the quantum Hall regime. Topological order was recently discovered in some three-dimensional materials, dubbed topological insulators, in zero magnetic field. Spin-orbit coupling, an intrinsic property of all solids, drives the formation of the topological state. The first part of the talk will explain how topological insulators were predicted and discovered by building on the quantum Hall effect. The second part will cover more recent work on connections between topological insulators, magnetoelectric effects ("axion electrodynamics"), and strong correlation effects.

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Electromagnetic Response of Weyl Semimetals

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Abstract

It has been suggested recently, based on subtle field-theoretical considerations, that the electromagnetic response of Weyl semimetals and the closely related Weyl insulators can be characterized by an axion term ŒE · B with space and time dependent axion angle ϑ(r, t). We construct a minimal lattice model of the Weyl medium and study its electromagnetic response by a combination of analytical and numerical techniques. We confirm the existence of the anomalous Hall effect expected on the basis of the field theory treatment. We find, contrary to the latter, that chiral magnetic effect (that is, ground-state charge current induced by the applied magnetic field) is absent in both the semimetal and the insulator phase. We elucidate the reasons for this discrepancy.

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Figure

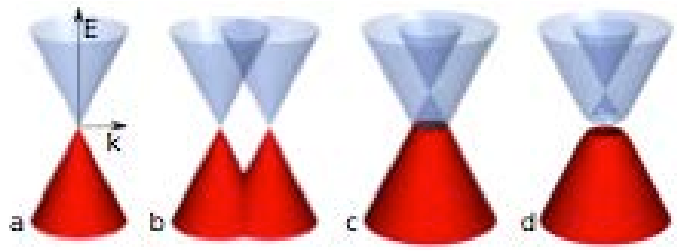

Figure Caption. Low energy spectra in Dirac and Weyl semimetals. a) Doubly degenerate massless Dirac cone at the transition from a TI to a band insulator. Weyl semimetals with the individual cones shifted in b) momenta and c) energy. Panel d) illustrates the Weyl insulator which can arise when the excitonic instability gaps out the spectrum indicated in c). In all panels two components of the 3D crystal momentum k are shown.

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Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Magnetoelectric coupling and surface anomalous Hall effect

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Abstract

In this presentation I will review some recent development in the theory of the linear magnetoelectric (ME) effect in solids. The main focus will be on the orbital-magnetization response to an applied electric field. Remarkably, this response contains a contribution which is purely geometric, in that it can be expressed solely in terms of the Berry potential and Berry curvature of the Bloch states in k-space [1,2]. Like the Berry-phase polarization, this term is only well-defined modulo a quantum of indeterminacy. While the bulk polarization produces a bound surface charge, the geometric ME response gives rise to a surface Hall conductance, which in strong topological insulators amounts to half a quantum of conductance. In conventional magnetoelectrics the geometric term is not quantized, and gives only part of the orbital ME response [3]. Ab initio calculations of the linear ME coefficient will be presented for both topological (Bi2Se3) and conventional (Cr2O3) insulators [4,5].

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
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Interfacing 3D topological insulators with magnetism

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Abstract

Interfacing three dimensional (3D) topological insulators (TIs) with magnetism is expected to result in "exotic broken symmetry surface phases" that are of contemporary interest [1]. We describe experiments that use a panoply of techniques (ARPES, SQUID magnetometry, FMR, neutron reflectivity and magnetotransport) to probe the nature of ferromagnetic order at the surface and in the bulk of epitaxially grown, magnetically doped Bi chalcogenide thin films [2,3]. Complementary to the direct magnetic doping of TIs, we also examine a different sample geometry [4] wherein a ferromagnetic insulator (FMI) is interfaced with a TI [4]. By studying the quantum corrections to the conductivity in FMI/TI transport devices, we reveal the effect of broken time-reversal symmetry on the surface state and show that the data are consistent with the predicted opening of a magnetic gap [5].

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Band gap opening and lifetime broadening of topological surface states with and without magnetic moments

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We study the lifetime broadening of the angle-resolved photoemission signal from the surface states of Bi_2Se_3 and Bi_2Te_3. It is revealed that hexagonal warping in Bi_2Te_3 introduces an anisotropy for electrons propagating along ΓK and ΓM. Moreover, we show that the electron-phonon coupling strength is substantial and in good agreement with theoretical predictions. In addition, we find that Fe surface impurities have a much stronger influence on the lifetimes as compared to Ag. This conclusion is possible because we deposite the Fe a low temperature where it is slightly p-doping and, therefore, does not introduce extra scattering channels due to increased warping or due to the bulk conduction band.

Angle-resolved photoemission experiments shows that Fe deposition does not open a surface band gap in Bi_2Se_3 and Bi_2Te_3 up to large deposited Fe amounts equivalent to one monolayer. When the magnetic moment is instead introduced into the bulk of Bi_2Se_3, large band gaps occur at the Dirac point, as is shown for $(Bi_{1-x}Mn_x)_2Se_3$. However, these are an order of magnitude larger than predicted by density functional theory for comparable systems and do not change with temperature from 10 K to room temperature. SQUID and x-ray magnetic circular dichroism shows that their origin is not related to ferromagnetic order of volume or surface of $(Bi_{1-x}Mn_x)_2Se_3$. Moreover, Mn deposited directly on pure Bi_2Se_3 does not open a band gap which calls also an important role of the local Mn magnetic moment into question. This problem is discussed in view of recent theoretical approaches.

Finally, we discuss the spin polarization and the circular dichroism in angle-resolved photoemission. The topological surface states show a strong circular dichroism which has been explained in the literature as being due to either the initial-state spin angular momentum, the initial-state orbital angular momentum, or the handedness of the experimental setup. All of these interpretations conflict with our data from Bi_2Te_3 and Bi_2Se_3 which depend on the photon energy and show several sign changes. This assigns the dichroism to a final-state effect which is confirmed by one-step photoemission calculations coupled to ab initio theory. However, the spin polarization of the photoelectrons remains a reliable probe for the spin in the initial state.

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Tailoring the electronic texture of a topological insulator via its surface orientation

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Abstract
Topological insulators are characterized by an insulating bulk band structure, but topological considerations require their surfaces to support gap-less, metallic states. Meanwhile, many examples of such materials have been predicted and found experimentally, but the experimental effort has usually concentrated on one particular surface orientation (usually (111)) of a given material. Here we realize a different surface termination, (111), for the topological insulator $Bi_{1-x}Sb_x$ ($x \approx 0.15$). Apart from confirming the basic topological prediction that the bulk crystal is, in fact, enclosed by metallic surfaces, this permits us to engineer the number topologically protected Dirac cones on the surface. In this case, we obtain three Dirac cones instead of one. We also discuss the more general issue of topological protection of surface states on topological insulator and semimetal surfaces.

Acknowledgements.

This work is supported by the VILLUM foundation.

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Probing spin textures of topological surface states in ternary chalcogenides

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Three-dimensional topological insulators (3D TIs) with a gapless topological surface state (TSS) in a bulk energy gap induced by a strong spin-orbit coupling have attracted much attention as key materials to revolutionize current electronic devices. A spin helical texture of a TSS, where the electron spin is locked to its momentum, is a manifestation of a 3D TI.

A number of well-known thermoelectric and phase-change materials have so far been predicted to be 3D TIs. In order to experimentally confirm their topological natures, spin- and angle- resolved photoemission spectroscopy (SARPES) is one of the most powerful tools and it has actually been playing major roles in finding some real 3D TIs [1, 2]. Among the established 3D TIs, Bi_2Se_3 has been most extensively studied because of its relatively large energy gap and the simplest TSS. However, the topological surface state is energetically obscured by bulk continuum near and below the Dirac point, which is disadvantageous for spintoronic applications.

SARPES experiments were performed at the ESPRESSO end station attached to the APPLE-II type variable polarization undulator beam line (BL-9B) at Hiroshima Synchrotron Radiation Center (HSRC) [3]. The VLEED-type spin detector utilized in the ESPRESSO machine achieves a 100 times higher efficiency compared to that of conventional Mott-type spin detectors [2]. Photoelectron spin polarizations are measured by switching the direction of in-plane target magnetizations, thereby simultaneously eliminating the instrumental asymmetry, which is a great advantage for a quantitative spin analysis of nonmagnetic systems such as 3D TIs.

In this talk, some of the ternary 3D TIs such as $TlBiSe_2$ [4], $GeBi_2Te_4$ [5], Bi_2Te_2Se, and Bi_2Se_2Te [6] are shown to possess TSSs with marked spin polarizations. It has been revealed for $GeBi_2Te_4$ that a disorder in the crystal has a minor effect on the surface-state spin polarization, which is ~70% near the Dirac point in the bulk energy gap region (~180 meV). Highly spin-polarized features are also found for Bi_2Te_2Se and Bi_2Se_2Te, which are persistent across the Dirac point. The availability of both upper and lower TSSs promises to extend the variety of spintoronic application, for instance, to dual gate TI devices and topological p-n junctions.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Surface states of Sn ultrathin films with Dirac-like dispersion and helical spin polarizations

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Abstract

The growing interest on topological insulators (TI) comes from their various exotic electronic phenomena, such as robust Dirac cones made by surface states with helical spin and orbital polarization and dominance of 3D bulk electronic properties with respect to the 2D surface electronic structure [1]. Since the parity eigenvalues of 3D bands are the key properties that determine the topological order (TO) of the material, which categorize semiconductors as non-trivial TI or trivial insulators, material design based on the theoretical calculations of 3D band structures have achieved a great success [2]. However, in parallel to such a bulk-based method, there are other ways to elaborate topological materials, that are the manipulation of the 3D band structure by structural strain [3] or quantum size effect [4].

In this work, we have grown ultrathin α-Sn films which have a diamond-type atomic structure on lattice-matched InSb substrates. α-Sn has an inverted band structure with a non-trivial TO [5], but the surface states of Sn have gathered less attention because they are unstable up to room temperature and the bandgap in the bulk bands is absent due to the degeneracy between light-hole (LH) and heavy-hole (HH) bands. However, MBE-grown α-Sn film is stable even up to 250 C and the ultrathin thickness (up to ~50 ML) could open a 3D bandgap (see Figure A).

Figure B shows an angle-resolved photoelectron spectroscopy (ARPES) map measured on a Sn(001) film. A surface state is observed which shows almost linear dispersion, suggesting a Dirac-cone-type nature of this state. The surface state also shows circular dichroism and clear spin polarization as measured with spin-resolved ARPES with a spin Mott detector. Both of them are consistent with a helical spin and orbital polarization which are characteristic of the Dirac cone of surface states on TI. Thus, we conclude that we could fabricate a new TI phase in ultrathin films.
In the presentation, a comparison with theoretical calculation and evolutions of the surface state with film thicknesses will also be discussed.

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Figure

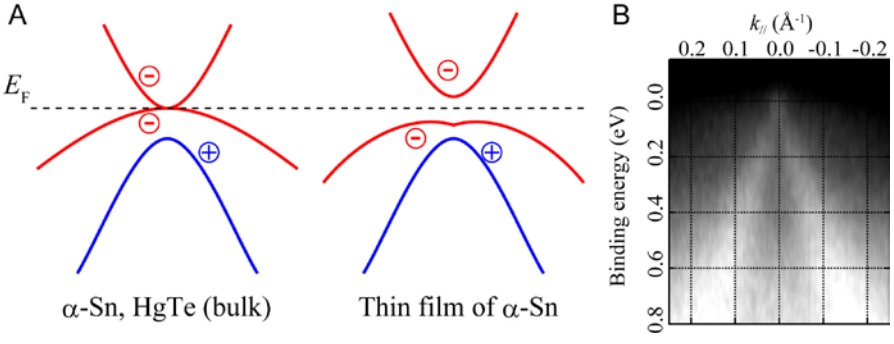

Figure Caption. A) Schematic pictures of 3D band dispersions of heavy diamond-type elements. **B)** Band dispersion of a Sn(001) film measured with ARPES. The thickness is estimated to be 20 monatomic layers.

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High Quality Synthetic and natural topological insulators

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Abstract

Topological insulators (TIs) are attracting increasing attention owing to their peculiar helical states at their boundaries. However, electrical detection of these states is complicated by the interference of bulk conduction that arises due to pronounced doping originating from lattice defects. We have demonstrated the growth of high quality nanoplatelets of the topological insulator Bi_2Te_2Se through van der Waals epitaxy on thin hexagonal boron nitride (hBN) substrates [1]. In this manner, a significant increase of the surface state carrier mobility is achieved, thus opening the possibility to observe well-developed Shubnikov-de Haas oscillations in the platelets. Furthermore, the platelet's small thickness enables effective tuning of the Fermi level position with the aid of a back gate.

High quality TIs cannot only be synthesized in the laboratory but can also be found in nature. We have found that the mineral Kawazulite with the general chemical composition $Bi_2(Te,Se)_2(Se,S)$ is a natural TI whose electronic properties compete well with its synthetic counterparts [2]. Based on this discovery, natural TIs may exist in other minerals, which due to their minimized defect densities display even better electronic characteristics.

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Some recent results in MBE grown 3D topological insulators

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Abstract

In this talk, I will first report the successful growth of Bi_2Se_3 (221), a high-index epifilms, by molecular-beam epitaxy (MBE). Angle-resolved photoemission spectroscopy (ARPES) measurements reveal the Dirac cone structure of surface states on such a high-index Bi_2Se_3 surface. The Fermi surface is elliptical, suggesting anisotropy along different crystallographic directions. Anisotropic transport is investigated in high index (221) topological insulator Bi_2Se_3 films. The observed nonlinear Hall effect at high temperatures reveals the existence of a high mobility conducting channel in addition to the ordinary bulk one. In the presence of this high mobility channel, a non-saturating linear magneto-resistance (LMR) is observed in high magnetic fields. The localization of the high mobility channel at low temperatures suggests the non-topological nature of the channel and the important role of disorder in the transport properties of these high index films. The asymmetry of LMR with respect to the field direction further indicates the disorder-induced admixture of Hall signal in the MR measurement. All these results reveal that the observed LMR is unlikely of quantum origin, but from the disorder effect as proposed by the classical Parish-Littlewood model. Secondly, I will report the growth of $Fe_{1+x}Te/Bi_2Te_3$ bilayers via a solid state chemical reaction scheme using MBE technique. Transport characterization based on the four-probe method shows that the as-grown $Fe_{1+x}Te$ layer undergoes fully superconducting transition at temperature around 12K, and the zero resistance was achieved around 6K. Electric transport data provides evidence that the magnetic clusters induce spontaneous vortices. The temperature dependence of the resistance reveals complex flux dynamics with all the characteristics of a second-order vortex melting from a low-temperature vortex glass to a liquid vortex phase, which is usually only observed in finite applied magnetic fields. Evidence on the ferromagnetic source at the bilayer will be discussed.

Acknowledgements.

This work is partially supported by the Research Grants Council of Hong Kong Grants SEG_HKUST03, SEG_CUHK06, 706110, 706111, 604910, 605011, 603010 and 605512.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

A 2D TI in various crystal-chemical surroundings: A study on the bismuth bilayer

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Abstract

A corrugated bismuth layer – the building unit of the elemental bismuth structure – was recently predicted to be a topological insulator [1]. Using a 2D tight-binding model, *Murakami* demonstrated that such a corrugated honeycomb-like $[Bi_2]$ layer has only one pair of helical edge states and an odd, non-trivial Z_2 topological invariant. Moreover, this state remains non-trivial even if the inversion symmetry of the bismuth layer is broken, e.g. in a heterostructure or in case of a bismuth thin film on a substrate. Oriented bismuth films are being intensively studied for an experimental proof [2], while we take a complementary approach and seek candidate TIs in compounds with a single corrugated bismuth layer $[Bi_2]$ as a structural fragment [3].

Layered compounds with such a fragment are plentiful. We have analyzed the electronic structures of two groups: 1) bismuth iodides built by stacks of $[Bi_2]$ terminated by iodine atoms; 2) layered Bi_nTeI compounds built by a stacking of infinite $[Bi_2]$ and BiTeI [4] layers with various alternation sequences, e.g. $Bi_2TeI = [Bi_2]\cdot 2[BiTeI]$ and $Bi_3TeI = [Bi_2]\cdot[BiTeI]$.

The band structures were calculated using the Full-Potential Local-Orbital (FPLO) code [5]. The calculation of Z_2-invariants for systems with an inversion center was implemented following the formalism of *Fu* and *Kane* [6].

Generally, a 2D TI forming a crystal structure with other building units either keeps its topological properties, resulting in a 3D weak TI or even a strong 3D TI, or it turns into a trivial metal/insulator owing to interactions with the other fragments. In our study, bismuth iodides are found to be trivial insulators, whereas Bi_2TeI is found to be a new 3D weak TI with the topological invariants 0;(0,0,1). Bi_3TeI is found to be a poor metal that could become a strong topological insulator under *p*-doping. The impact of increasing polarity on the abovementioned electronic structures upon chemical substitutions of selenium for tellurium and bromine or chlorine for iodine is considered.

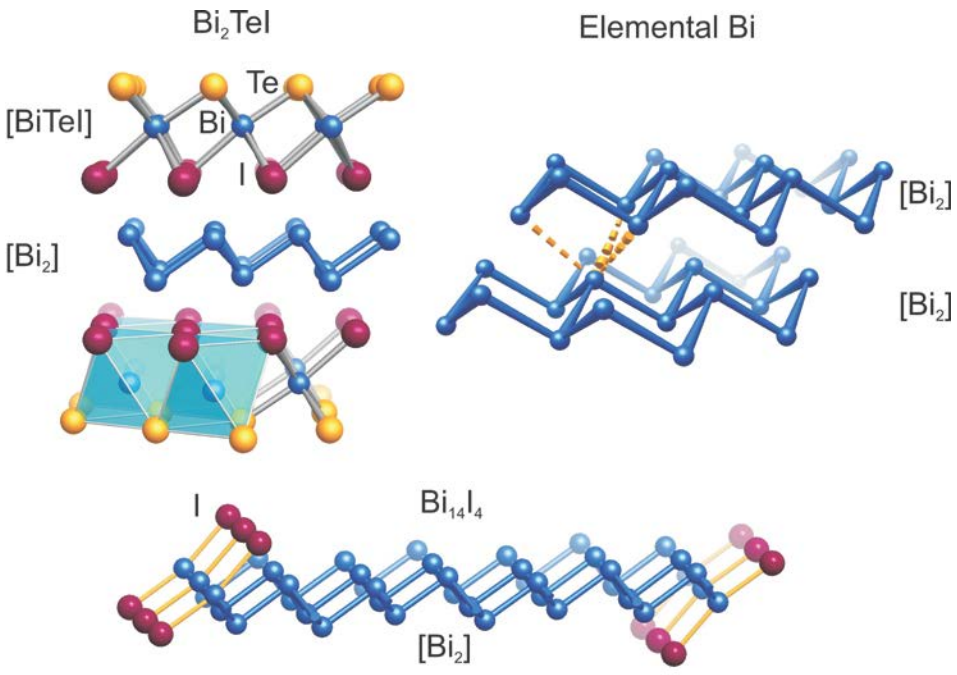

Figure 1. A corrugated honeycomb-like [Bi_2] bilayer in selected crystal structures.

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Acknowledgements

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

BiTeI: a high-pressure topological insulator?

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Abstract

Giant Rashba-type spin splitting of bulk states occurs in BiTeI, a non-centrosymmetric layered semiconductor [1]. Intriguingly, at high pressures, BiTeI is expected to become a topological insulator [2]: applying pressure will close the band gap and reopen it, with inverted conduction and valence bands. Large spin-orbit interaction lies behind both giant Rashba spin splitting (the largest such effect observed in a bulk compound), and the unusual surface states in topological insulators. It is therefore very interesting to see how these two different manifestations of spin-orbit interactions take place in the same material. Yang et al [2] predict that applying hydrostatic pressure will increase the Rashba splitting, close the band gap and cause a quantum phase transition at a critical pressure Pc, with unconventional metallic behavior. Above a critical pressure Pc, the band gap reopens but the conduction and valence band states are now inverted; BiTeI should thus become a topological insulator. Because the inversion symmetry is absent, the Dirac states are expected to have different shapes on different sides of the material.

To understand the nature of the high-pressure phase by probing the band structure of BiTeI under pressure, we embarked upon a study of the high-pressure optical properties, transmission and reflectivity of BiTeI up to 15 GPa. At low pressures, a metallic contribution to the conductivity of BiTeI is caused by charged impurities, with a well-defined plasma edge signifying coherent transport. Combining reflectivity and transmission under pressure, we see that the gap strongly shifts toward lower energies as pressure increases, followed by a very steep decrease at 9 GPa. At 10 GPa, the gap seems to collapse, and we identify this pressure with the critical pressure Pc. Above 12 GPa, the reflectivity level increases again in the low energy region. However, the allure of the reflectivity curves is different from the low-pressure reflectivity. This points to a different nature of the high-pressure ground state of BiTeI. We discuss the possible signatures of topological surface states in the high-pressure phase of BiTeI.

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Acknowledgements

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

X-ray absorption spectroscopy of magnetic atoms coupled to TI surface states

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Abstract

The talk focuses on potentials of X-ray Absorption Spectroscopy (XAS) techniques in the field of topological insulators coupled to magnetic degrees of freedom.
As an example an extensive study of magnetic and electronic properties of magnetic atoms on bulk topological insulators is presented, using both local low-temperature Scanning Tunneling Microscopy and Spectroscopy (STM and STS) and non-local XAS [1].
Iron sub-monolayer coverages in the regime between 0.5% and 20% are deposited at low temperatures in order to minimize diffusion on the surface. With low-temperature STM we observe that Fe atoms adsorb in two different hollow-site positions which can be topographically distinguished and have unique spatial electronic signatures.
X-ray magnetic circular dichroism (XMCD) measurements in the Fe coverage range <1% indicate a high-spin configuration of these iron impurities and the magnetic easy axis is found to be in-plane. The magnetic properties and shape of the XMCD-spectra will be interpreted in terms of *ab-initio* density functional theory which suggests a strong hybridization of the in-plane *d* -orbitals with the environment.
With increasing Fe coverage changes in the spectral shapes as well as the magnetic properties are observed, which will be discussed in terms of an increasing coordination between Fe atoms.

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ERC Advanced Grant ‘‘FURORE’’, and North-German Supercomputing Alliance (HLRN).

Figure

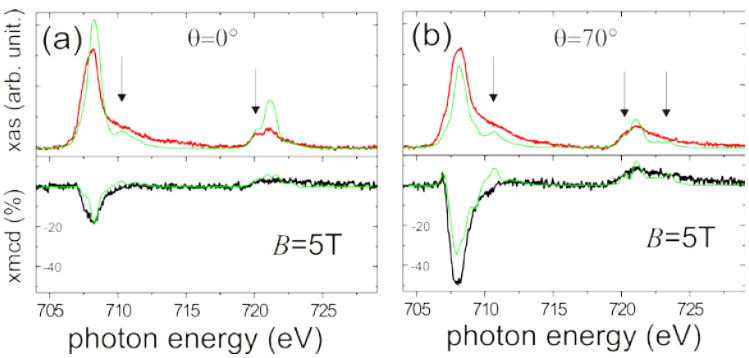

Figure: L3,2 XAS / XMCD example spectra of single Fe atoms on Bi2Se3 in (a) polar and (b) grazing geometry

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Effects of magnetic impurities on topological surface states

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Abstract

We study effects of magnetic impurities on topological surface state of Sb (111) surface by using first-principles density-functional method. The spin-orbit interaction is implemented into the SIESTA code in a form of additional fully non-local projectors, and supercells are used to calculate surface band structures. We consider Fe and Mn impurities at interstitial sites and substitutional sites near the surface. To analyze effects of impurities on the topological surface states, we simulate ARPES spectra and obtain projected density of states of impurities near the Fermi level. We find that Fe and Mn impurities have significant local magnetic moments near the Sb surface, and their effects on the dispersion of the surface states depend strongly on the impurity sites. We discuss scattering mechanism of the surface states by the impurities and its implication on the ordering of impurity magnetic moments.

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Acknowledgements.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

How to detect and braid Majorana fermions in a quantum spin Hall insulator

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Abstract

We show how a quantum dot with a ballistic single-channel point contact to a superconductor can be created by means of a gate electrode at the edge of a quantum spin Hall insulator (such as an InAs/GaSb quantum well). A weak perpendicular magnetic field traps a Majorana zero-mode, so that it can be observed in the gate-voltage-averaged differential conductance as a zero-bias peak. The one-dimensional edge does not permit the braiding of pairs of Majorana fermions, but this obstacle can be overcome by coupling opposite edges at a constriction, allowing for a demonstration of non-Abelian statistics.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Majorana Single Charge Transistors

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Abstract

Topologically nontrivial insulators and superconductors exhibit many remarkable non-local features such as teleportation or non-Abelian statistics. For a one-dimensional topological superconductor wire, such effects can be traced back to the existence of zero-energy Majorana bound states (MBS) localized at each end of the wire.
While big efforts have been devoted to explore the conditions for the presence of MBS in hybrid nanostructures, little attention has been paid to the effect of electron-electron interactions which are always unavoidably present.
In this presentation I shall discuss an interacting variant of the previously studied Majorana wire set-up which wecall Majorana Single Charge Transistor. Interactions are described in terms of a finite charging energy and we study its effects on the transport properties through the MBS system. We have analyzed the regime of weak [1] and strong[2] Coulomb blockade showing the emergence of oscillations as a function of the gate voltage and the crossover from resonant Andreev reflection to the electron teleportation regimes. We further show that the current can be expressed in terms of a Landauer-Buttiker type formula valid for arbitrary charging energy. Side band peaks in the differential conductance, tunable by the Josephson coupling to an external superconducting lead provide a unique signature of the presence of MBS in the system.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Ac Josephson effect and Multiple Andreev Reflection currents in nanowire junctions with Majorana fermions

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Abstract

Recent experiments [1-3] have reported conductance measurements in semiconducting nanowire-based systems that support the existence of Majorana bound states (MBS)s at normal-superconductor (NS) junctions. Although these experiments are partially consistent with the Majorana interpretation [4], other mechanisms such as disorder [5], Kondo physics [6], or even Andreev bound states [7] cannot be completely ruled out. It is thus extremely desirable to study further effects that might provide smoking gun signatures for topological superconductivity and Majorana fermions. In this talk, I will discuss how the ac Josephson current in voltage-biased SNS junctions with nanowires in the topological phase contains anomalously long-lived transients that provide unequivocal proof of the existence of MBSs [8]. The multiple Andreev reflection (MAR) currents in such junctions also exhibit unique features related to topology, such as the gap inversion, the formation of MBSs, and fermion-parity conservation. Moreover, the critical current, which remarkably does not vanish at the critical point where the system becomes gapless, provides a direct trace of the topological transition [9].

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Figure

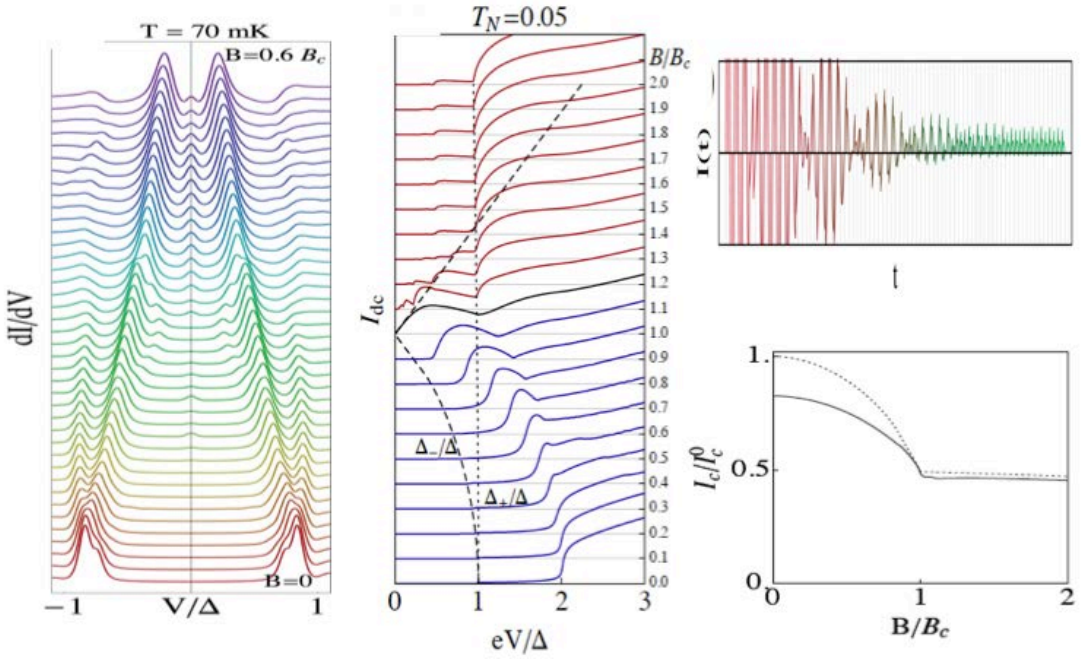

Figure Caption. Left: dI/dV of a NS nanowire junction for increasing magnetic fields (bottom to top). At the topological transition, a zero-bias anomaly emerges owing to Majorana bound states formation. The closing of the topological gap is not visible, which is consistent with the experimental observations (adapted from [4]). Center: MAR current of a SNS nanowire junction in the tunneling regime. The steps at eV=2Δ clearly show the closing of the topological gap. When the gap reopens, the steps locate at eV=Δ owing to the emergence of Majorana bound states (adapted from [9]). Right top: Ac Josephson current of a SNS nanowire junction which presents a typical dissipative decay from the nontrivial fractional regime into the stationary MAR regime (adapted from [8]). Right bottom: the critical current of a SNS nanowire junction provides a direct trace of the topological transition (adapted from [9]).

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Entropy transport in Bi_2Se_3 and Bi_2Te_3

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Abstract

Bi_2Se_3 and Bi_2Te_3 are well know compounds in the thermoelectricity community since they realize a high figure of merit [1]. More recently this compounds have been proposed as a host of a new class of quantum state of matter, namely topological insulator [2]. However due to the anti-site defects or charged vacancies, Bi_2Se_3 and Bi_2Te_3 are low carrier concentration bulk systems.

Motivated by their high thermoelectric response, we start to explore the electronic grounds state of Bi_2Se_3 and Bi_2Te_3 with a bulk carrier concentration from n= $10^{19}cm^{-3}$ to $10^{17}cm^{-3}$ by entropy measurement. In this presentation we will report our measurement of the thermopower and the Nernst effect down to 300mK and up to 34T [3]. We can resolved, as in the case of bismuth and graphite [4,5], significant quantum oscillations in thermoelectricity response. A comprehensive analysis of the Landau level spectrum of both systems will be proposed.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Topological Insulators – What can we do with ultracold atoms

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Abstract

I will present a review of recent efforts to quantum engineer, create and manipulate various kind of topological insulators in systems of ultracold, atoms. Particular attention will paid to possibilities of detection of edge states and measurements of topological invariants.

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POSTERS

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Origin of Rashba-splitting in the quantized subbands at Bi_2Se_3 surface

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Abstract

The recent observation of a topologically protected surface state (TSS) in Bi_2Se_3 [1] marked the discovery of a model system for 3D topological insulators (TIs) and has lead to a surge of renewed interest in the properties of this material. The Bi_2Se_3 (111) surface hosts within the bulk bandgap a single TSS with Dirac cone dispersion and possesses a helical character, which infers a defined spin polarization for a particular momentum value [1-3]. It has already been shown that the modification of the Bi_2Se_3 surface with non-magnetic adsorbates does not alter TSS protection [1,5–7]. However, it dopes the TSS and can even change surface electronic properties. Surface *n*-doping creates two sets of new states at the surface, which appear simultaneously in the immediate vicinity of the TSS within the projected bulk conduction band (CB) and valence band (VB) regions. While parabolic bands with a large Rashba splitting are observed above the Dirac point, the bands below are M-shaped, can overlap with the TSS, and do not show a clear spin splitting. These two band sets have been mainly interpreted as quantized subbands resulting from the confinement of a pair of two dimensional electron gases (2DEGs) at the surface created via CB and VB bending [6-9]. Practically, the largely spin-split bands add a new feature to Bi_2Se_3 surface for spintronic applications [8]. However, the reason behind the discrepancy in Rashba splitting between CB and VB subbands is not clear. Here, by analyzing recorded surface band structures using angular resolved photoemission spectroscopy (ARPES) from differently treated Bi_2Se_3 surfaces we examine the formation of the M-bands and their overlap with the TSS via band bending. We show that the potential gradients at both 2DEGs are similar (see figure below) and therefore not responsible for the splitting discrepancy. On the other hand, our first principles calculations show that the contribution of Bi 6*p* states to VB is clearly smaller than to CB. Therefore, and since Bi 6*p* states are characterized by a strong spin-orbit coupling (SOC), we attribute the spin-splitting discrepancy to a difference in SOC strength.

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Acknowledgements

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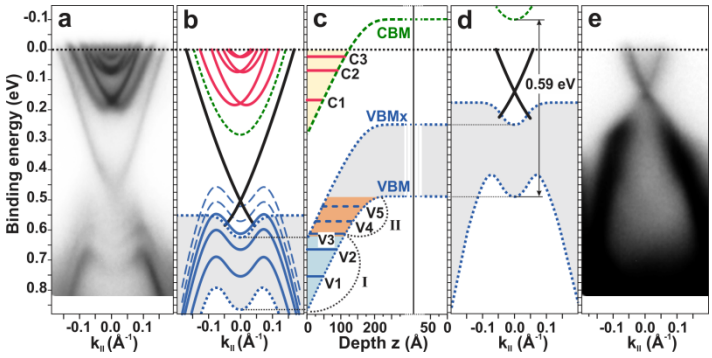

Figure Caption
Sketch of surface bending of CB and VB and the formation of quantized CSBs and VSBs. **a.** Experimental band structure (Fig.1.c). **b.** Schematic outline of a. **c.** Representation of the surface with (left) and without (right) surface band bending at $k_{//} = 0$ Å^{-1} **d.** schematic outline of e. **e.** experimental band structure directly after crystal cleaving in vacuum**.**

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Landau Levels and Edge States at the Surface of a Topological Insulator.

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Abstract

A topological insulator, TI, is a material, which is gapped in the bulk but has gapless states at the surface. On strong topological insulators the electrons at the surfaces are described by a massless Dirac equation, and the band structure is a Dirac cone located at the centre of the two-dimensional Brillouin zone.
A magnetic field, B, applied perpendicular to the surface will lead to Landau levels in the electronic spectrum and eventually to the quantum Hall effect. The Landau levels occurs at energies $E_n=\pm(2n)^{1/2}\, v\, l^{-1}$ where v_F is the velocity of the surface states, l is the magnetic length and n=0,1,2.. Since the Hall conductivity increases by e^2/h where the Fermi energy cross a Landau level, the Hall conductivity in an isolated surface of a TI is half quantized, $\sigma_{xy}= (n+1/2)\, e^2/h$.

In this presentation we discuss the chiral edge states associated with the half-integer quantum Hall effect. The chiral edge states can only be integer quantized, and the conflict between the integer chiral edge states and the half-integer quantum Hall effect should be resolved by considering a slab geometry. In this configuration the top and bottom surface states should necessary talk through the chiral two-dimensional Dirac-like electron gas that reside on the perpendicular surface connecting them.
We study a quantum wire along the y-direction, with a rectangular section. By imposing the appropriated boundary conditions we obtain the Dirac equations describing the motion of the electrons in the different planes of the wire.
In presence of a magnetic field applied in the z-direction, electrons in the x-y planes move in cyclotron orbits whereas electrons in the y-z plane are not affected by the orbital magnetic field. At the interface between these planes chiral edge states should appear. In this presentation we discuss the nature of these edge states, the coupling between edge states located in the top and bottom surfaces, the effect of Zeeman splitting on the edge states, the effect of a bias voltage, etc.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Inducing Topological Order in Graphene

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Abstract

While the quantum spin-Hall state was initially proposed in graphene, its experimental realizations have only been found in quasi two-dimensional quantum wells grown in semi-conductors. A recent proposal by C. Weeks *et al.* revived the interest of topological order in graphene by considering a strong spin-orbit interaction induced by the deposition of heavy adatoms such as Indium. In this talk, I will discuss some properties of the random topological insulator obtained in such a way. I will then consider the interplay between such a strong induced spin-orbit and an associated superconducting pairing. In particular I will discuss the possible appearance of exotic superconducting order in this system.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Multiple Andreev reflection and critical current across a topological transition in superconducting nanowire junctions

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Abstract

We study transport in biased Josephson junctions made of nanowires with strong spin-orbit coupling, as it transitions into a topological superconducting superconducting phase for increasing Zeeman field.

Despite the absence of a fractional steady-state ac Josephson current in the topological phase, the dissipative Multiple Andreev Reflection current at different junction transparencies is particularly revealing.

It exhibits unique features related to topology, such as the gap inversion, the formation of Majorana Bound States, and the fermion parity conservation. In contrast and rather surprisingly, the critical current does not vanish at the critical point where the superconducting gap vanishes, exhibiting a discontinuous instead. These results demonstrate the feasibility to probe the formation of Majorana states without the need of phase sensitive or noise-related measurements.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Single crystals growth of topological insulators in $Bi_2(Se_xTe_{1-x})_3$ and $Cd_xHg_{1-x}Te$ systems

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Abstract

Topological insulators have generated a great interest in the fields of condensed matter physics, chemistry and materials science. The topological insulator is an insulator in the bulk, while it conducts on the surface like a metal. Topological insulators occur as two-dimensional (2D) – also called quantum spin Hall state – and three-dimensional (3D) versions. They have a full energy gap in the bulk, but host topologically protected gapless edge (2D) or surface (3D) states [1, 2].

Single crystals of 3D topological insulators in the system $Bi_2(Se_xTe_{1-x})_3$, where x= (0.5; 0.75; 1) and 2D topological insulators in the system $Cd_xHg_{1-x}Te$ where x= (0; 0.025; 0.050; 0.075; 0.1) are grown by a vertical Bridgman technique.

The starting materials with high purity as follows Bi -99.999%, Se - 99.999%, Te- 99.9999%, Hg - 99.9999%, Cd - 99.9999% are mixed and placed in encapsulated quartz ampoules with diameter 20 nm for the Bi-based system and 10 mm for Hg – based system respectively. Furthermore, the crystals in the Bi-based system are additionally doped with Ca, Cu and Mn.

The possible reaction between Ca and quartz during the crystal growth of doped $Bi_2(Se_xTe_{1-x})_3$ is prevented by covering the inside surface of the quartz ampoule with pyrolytic graphite. The ampoules with walls thickness of 3.5 mm are used for Cd_xHg_{1-x} Te crystals growth due to the high vapour pressure of Hg (6-7 atm) and the danger of explosion. The $Bi_2(Se_xTe_{1-x})_3$ crystals are grown with a speed of 0.2mm/h and the ampoules rotation speed of 25 rot/min, while those of Cd_xHg_{1-x} Te with 0.07mm/h and 25 rot/min, respectively.

It is found that the Ca concentration reduced with the crystal length from 0.02% to 0.01% in the end of the crystal. The resistivity measured at temperature of 77K for Ca – doped $Bi_2(Se_xTe_{1-x})_3$ crystals is 2 times higher than those of Bi_2Se_3. XRD diffraction measurements are performed for all crystals compositions.

Figure Caption: Single crystals of Bi and Hg -compounds

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Electron-hole Cooper pairing fluctuations in thin film of a topological insulator

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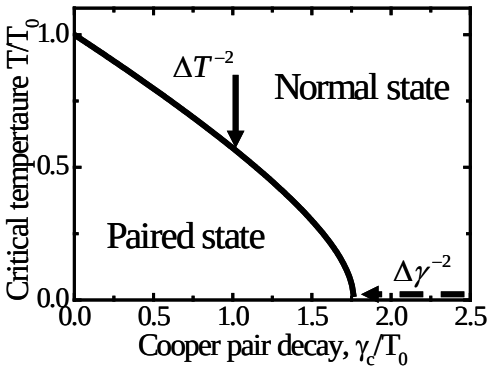
Abstract

We have considered the system of electrons and holes populating independently gated opposite surfaces of topological insulator thin film. Coulomb interaction between them can lead to electron-hole Cooper pairing [1,2] that is one of the realizations of topological superconductivity [3]. Also Cooper pairing leads to superfluidity, anomalies in drag effect and pronounced internal Josephson effect that manifests itself in colossal enhancement of tunnel conductivity [4].

We supposed that tunnel conductivity can be also enhanced by fluctuations of electron-hole Cooper pairing above critical temperature. Since fluctuations are increasing with decreasing of temperature one can expect considerable enhancement of tunnel conductivity in vicinity of critical temperature. The microscopic theory of the described effect is developed.



The phase diagram of the system in presence of disorder which strength is parameterized by Cooper pair decay γ_c is presented on the Fig. Here T_0 denote critical temperature without disorder. We showed that Cooper pair fluctuations lead to divergence of tunnel conductivity at critical temperature. In vicinity of classical phase transition (solid arrow on Fig) dependence of tunnel conductivity on temperature is critical one with critical index $\nu = 2$. In vicinity of quantum critical point (dashed arrow on Fig) dependence of tunneling conductivity on Cooper pair decay is also critical one with the same critical index $\mu = 2$. The predicted effect can be interpreted as fluctuation internal Josephson effect.

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Acknowledgements

The work was supported by RFBR project 12-02-31199 and by scholarship from Dynasty Foundation.

Figure

Figure Caption. Phase diagram of the spatially separated electrons and holes in thin film of topological insulator in presence of disorder.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Dirac-cone-like surface state in W(110): dispersion, spin texture and photoemission from first principles

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Abstract

We report on a theoretical study of a d_{z^2} surface state at the tungsten (110) surface, addressing in detail the spin-resolved electronic structure as well as photoemission spectroscopy. In agreement with recent experiments [1], this surface state shows a strongly anisotropic dispersion: In the H-Γ-H direction of the surface Brillouin zone, it disperses linearly but becomes flattened along the direction. The *ab initio* calculated spin texture agrees with the one derived from a model N-Γ-N Hamiltonian; due to two-fold surface symmetry and time-reversal symmetry, the out-of-plane spin polarization vanishes. The photoemission intensities depend sensitively on the polarization of the incident light, because of the orbital composition of the surface state. The photoelectrons become spin-polarized out-of-plane, which is attributed to breaking the time-reversal symmetry by the excitation process.

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We are very grateful to M. Donath (U Münster) and R. Feder (U Duisburg-Essen) for stimulating and fruitful discussions.

Figure

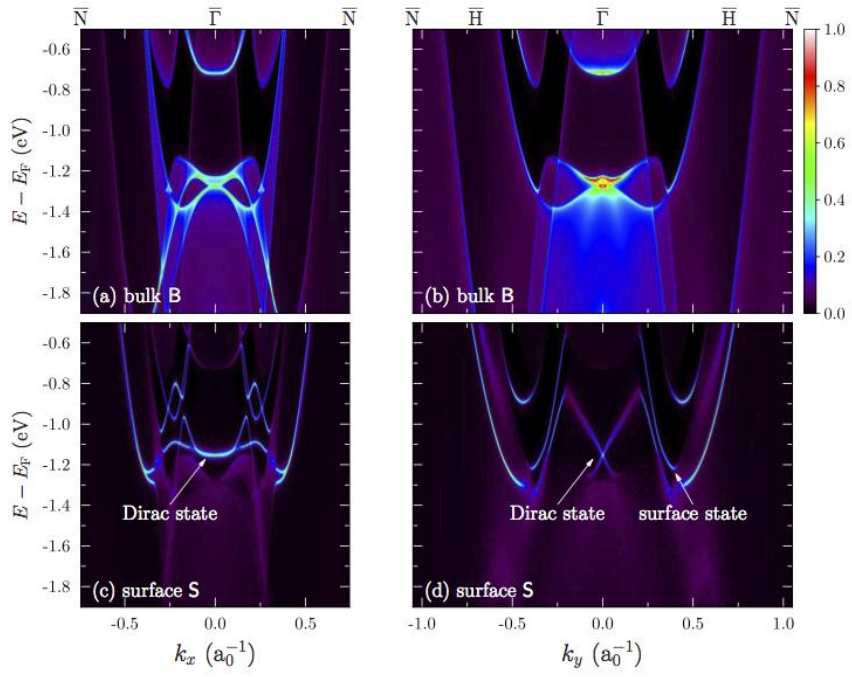

Figure Caption. Spectral density of a bulk layer B (top row) and the topmost surface layer S (bottom row) along the N–Γ–N (left column) and the N–H–Γ–H–N (right column) lines of the two-dimensional Brillouin zone. The spectral densities are normalized and, thus, share a common color scale (right of panel (b)). The Dirac state and a surface state are marked by arrows. The wavenumber k is given in inverse Bohr radii.

Workshop on NEW TRENDS in TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Influence of surface perturbations on the electronic structure of the topological insulator Bi_2Se_3

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Abstract

Topological insulators possess helical surface states that are protected by time reversal symmetry. Additionally, traditional surface states exist. The rich physics of these systems is determined by the actual boundary conditions at the surface which can distinctly be affected by adatoms. Using density-functional calculations, we investigate the influence of adsorbates and vacancies on the electronic structure of the Bi_2Se_3 surface.

First, the effect of an adsorbate induced two-dimensional electron gas at the surface is studied by adding a respective long-ranged potential *V(z)* to the self-consistent one. This simple approach already leads to a down-shift of the Dirac point and the appearance of additional Rashba-like surface states similar to the findings of various experiments [1, 2]. In addition to this, we observe several spin-split surface states emerging from bulk band edges in the unoccupied part of the band structure. These previously undescribed states are consistent with results of our inverse-photoemission experiments.

Secondly, our calculations show that monolayers of hydrogen or potassium adatoms give rise to long-ranged surface potentials and thus also induce the above mentioned features in the band structure. Furthermore, we find surface states that are specific to hydrogen and potassium, respectively. Selenium vacancies in the surface layer also cause long-ranged potentials and have similar effects in the band structure. The formation of long-ranged surface potentials can be explained by a charge rearrangement that is caused by the perturbation of the surface due to adatoms or vacancies, respectively. This effect is a specific feature of the layered structure of Bi_2Se_3. In the case of potassium adsorption on the Si(001) surface, for instance, we do not find a comparatively strong band bending at the surface.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Growth of High-Mobility Bi_2Te_2Se Nanoplatelets on hBN Sheets by van der Waals Epitaxy

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Abstract

The electrical detection of the surface states of topological insulators is strongly impeded by the interference of bulk conduction, which commonly arises due to pronounced doping associated with the formation of lattice defects. As exemplified by the topological insulator Bi_2Te_2Se, we show that via van der Waals epitaxial growth on thin hBN substrates the structural quality of such nanoplatelets can be substantially improved. The surface state carrier mobility of nanoplatelets on hBN is increased by a factor of about 3 compared to platelets on conventional Si/SiO_x substrates, which enables the observation of well-developed Shubnikov-de Haas oscillations. We furthermore demonstrate the possibility to effectively tune the Fermi level position in the films with the aid of a back gate.

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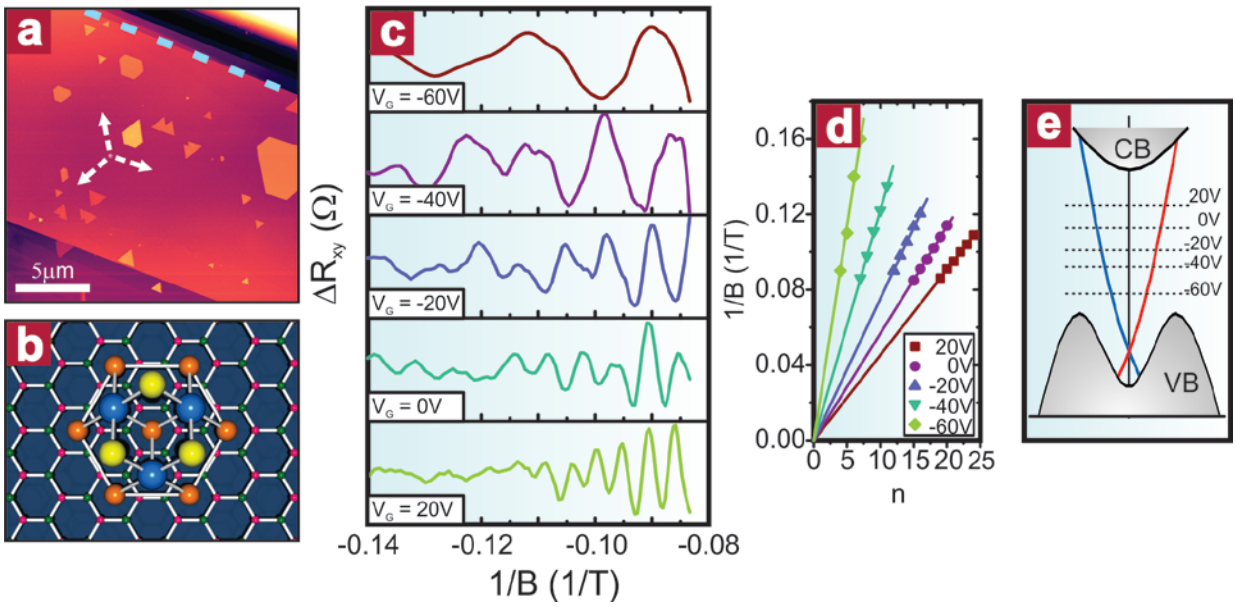
Figure



Shubnikov-de Haas oscillations in epitaxially grown nanoplatelets. (a) AFM image of Bi_2Te_2Se nanoplatelets grown on hBN. The armchair edges of the hBN sheet are marked in blue. (b) Schematic illustration of the proposed epitaxial growth mode on hBN. (c) Amplitude of the SdH oscillations as a function of 1/*B* for different back gate voltages. (d) Plot of LL index 1/*B* versus number of maximum for different gate voltages. (e) Sketch of the position of the Fermi level of the bottom surface in the Bi_2Te_2Se samples for different back gate voltages.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Impurity states in the quantum spin Hall phase in graphene

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Abstract

We consider the electronic properties of mid gap states, induced by a substitutional impurity, in otherwise boundless and perfect two dimensional graphene with a band gap open either by intrinsic orbit coupling, as described within the Kane and Mele model [1,2], or by sublattice inversion symmetry breaking. In the former case graphene is a non-trivial quantum spin Hall Insulator (QSHI) and in the later is a conventional insulator. The impurity potential shifts the on-site energy of a single atom by an amount V_0. When V_0 is sufficiently large, a midgap state bound to the impurity appears.

Using T-matrix theory with the full tight-binding model [3], we find [4] that the midgap states in the QSHI phase are different from those in graphene with a trivial band-gap on two counts. First, for equal V0 and bandgap, the binding energy of the midgap state is different for the two types of insulators. Second, and more important, in the QSHI midgap states carry currents whose quirality is determined by the spin and pseudospin of the residing electron, which is thereby endowed of an orbital moment. This effect is specific of the Quantum Spin Hall phase, i.e., is absent when a gap is open by means of sublattice symmetry breaking.

Our results suggest that exotic electronic states occur not only at the edges of the sample, but also around atomic scale defects, opening new ways to probe the electronic properties of topological insulators.

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Acknowledgements

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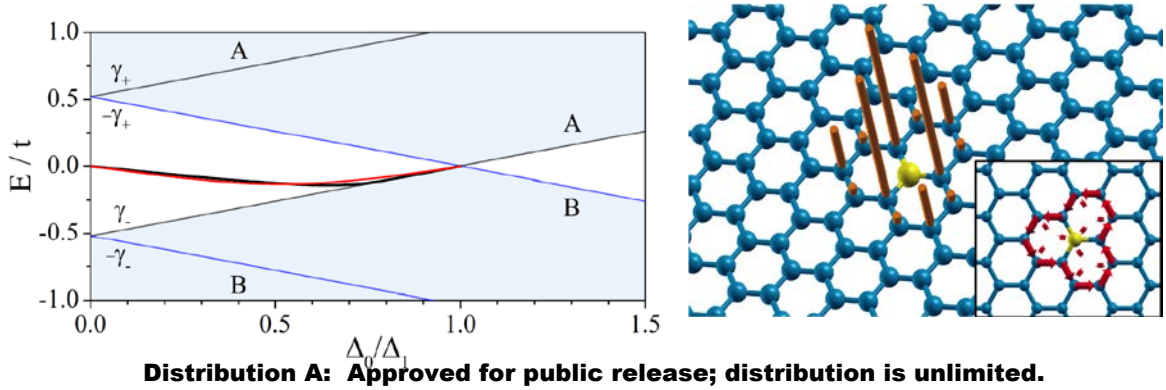
Figure

Figure Caption: Evolution of bands at K and K'. And in-gap impurity energy E_b, calculated with the lattice model (in black) and the continuum model (as a red line). **(R)** Local density of states as bars. The in-set shows the impurity-induced current between links for the state at E_b.



Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Electronic transport through disordered Bi(111) and Sb(111) ribbons and nanoconstrictions

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Abstract

In recent experiments of electronic transport in Bismuth nanocontacts we show the intriguing appearance of the quantum of conductance at room temperature. This unexpected finding can be explained in the context of the physics of topological insulators. Bismuth is a weak 3D topological insulator. However, a single bilayer of this material is a quantum spin Hall insulator. It was proposed [1] that bilayers can be exfoliated in formation process of the nanocontacts. Here we present the theoretical study of electronic transport in nanoribbons formed out of a single Bi(111) bilayer with constrictions (emulating the breaking process of these nanocontacts) and Anderson disorder. We find that only one out of the three conducting channels of a Bi bilayer survives in all cases. Moreover, the topologically protected channel is robust in presence of constrictions down to widths of a few atoms where inter-edge backscattering reduces the conductance below the quantum of conductance. This picture is highly robust against contraction and stretching of the lattice parameters. We compare these results with transport in Sb(111) nanoconstrictions.

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Acknowledgements

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Thermoelectric transport signature of the Bi_2Te_3 surface state

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Abstract

Bulk Bi_2Te_3 and related heterostructures are well known as efficient thermoelectric materials [1,2]. Recent research revealed Bi_2Te_3 to be a strong topological insulator, i.e. its bulk is insulating, while its surface is metallic due to the presence of robust gapless surface states [3]. While the spin structure and the low-temperature electrical transport gained much attention, the physics of the thermoelectric transport is still under debate. To contribute on this, we studied the electronic structure of the Bi_2Te_3 surface with a fully relativistic screened Korringa-Kohn-Rostoker Green's function method. The thermoelectric transport properties were calculated within the relaxation time approximation of the Boltzmann theory. The influence of temperature and doping on the thermoelectric transport were analyzed in detail and clear signatures of the surface state in the total thermoelectric transport can be revealed up to room temperature.

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Acknowledgements

This work is supported by the German Research Foundation within the Priority Program 1386: "Nanostructured Thermoelectric Materials: Theory, Model Systems and Controlled Synthesis".

Figure

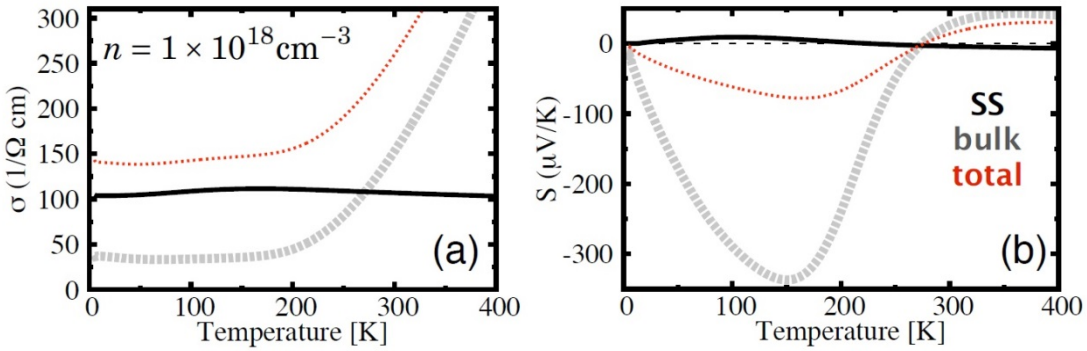

Figure Caption. Calculated temperature-dependent (a) electrical conductivity and (b) thermopower for slightly electron-doped Bi_2Te_3. The contributions of the metallic surface state (black solid line) and the semiconducting bulk states (grey dashed lines) to the total thermoelectric transport of the thin film (red dotted line) are given in detail.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Band bending in the unoccupied electronic structure of the topological insulator Bi_2Se_3

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Abstract

We report on angle- and spin-resolved inverse photoemission measurements on the topological insulator Bi_2Se_3. Vacancies and adsorbates on surfaces of topological insulators are known to modify the charge density at the surface [1,2]. The resulting band bending leads to an energetic shift of the band structure and the evolution of Rashba-split quantum-well states [3]. With regard to possible future applications, the influence of this band bending on the unoccupied electronic structure plays an important role. Here, we examine the time evolution of the band structure for two different sample systems of Bi_2Se_3: A thin film, MBE-grown on a Si(111)-substrate, and a bulk crystal. Especially the evolution of new structures due to the band bending will be discussed on the basis of theoretical calculations. Additionally, we investigate the influence of the threefold crystal symmetry, which causes differences between the electronic states in $\overline{\Gamma}\,\overline{M}$ - and $\overline{\Gamma}\,\overline{M}'$-direction.

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Figure

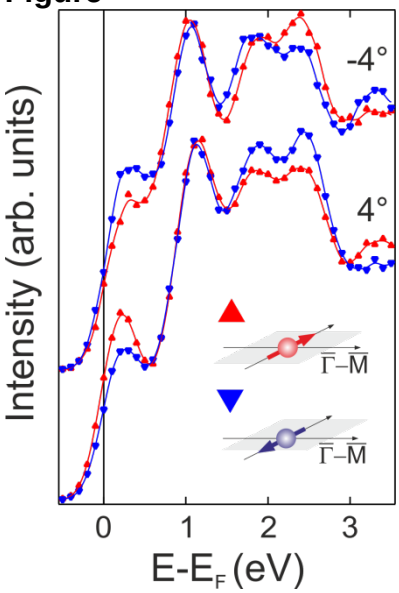

Figure Caption: Spin-resolved inverse photoemission spectra of the Bi_2Se_3 bulk crystal around $\overline{\Gamma}$, taken at -4° and +4° angle of incidence.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Probing topological states of phase change alloys by photoemission spectroscopy

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Abstract

Using spin- and angle-resolved photoemission spectroscopy (ARPES), we map the electronic structure and spin texture of the surface states of the topological insulator Sb2Te3 [1]. In addition to topological properties with a single spin-polarized Dirac cone around the Γ point, a strongly spin-orbit split surface state is observed at lower energy (Fig. a). DFT calculations reveal that the band is located within a spin-orbit gap in Γ-K direction. This is in accordance with a general argument requiring the existence of a surface state inside a spin-orbit gap in the interior of the Brillouin zone [2]. Thus, similar to the topological state, this state is protected by symmetry. Furthermore, epitaxially grown films of Ge2Sb2Te5 have been investigated. In scanning tunneling spectroscopy, a band gap of ≈0.4 eV is observed. Interestingly, the ARPES band structure reveals a prominent bulk valence band which crosses *E*F, forming maxima away from the Γ point (Fig. b). According to recent DFT calculations [3], this is a hint for a spin-orbit induced band inversion which is a requirement for topological properties.

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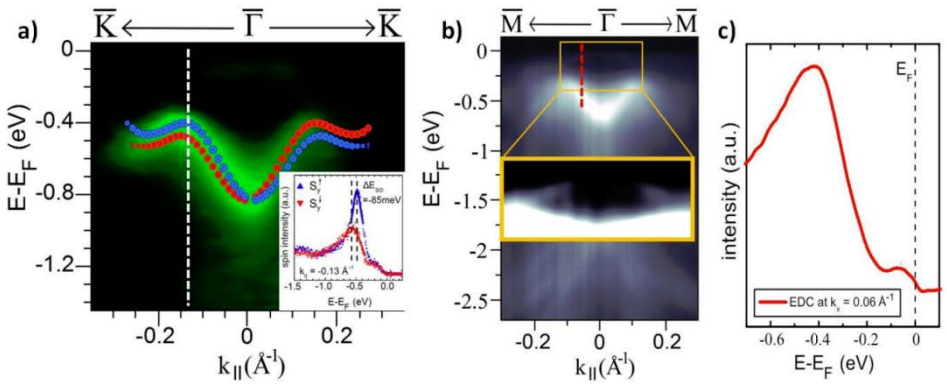

Picture Caption: a) Dispersion of the Rashba-type surface state measured by ARPES, superimposed with DFT calculation as blue and red dots; the dashed line marks the position of the spin-resolved energy distribution curves (EDC) in the inset. b) ARPES data of Ge2Sb2Te5 (111) with the onset of a state starting from the top of the bulk valence band (inset). c) EDC at the position marked in (b). All data at hv=22 eV.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Controlled growth and transport measurements of topological insulator nanostructures

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Abstract

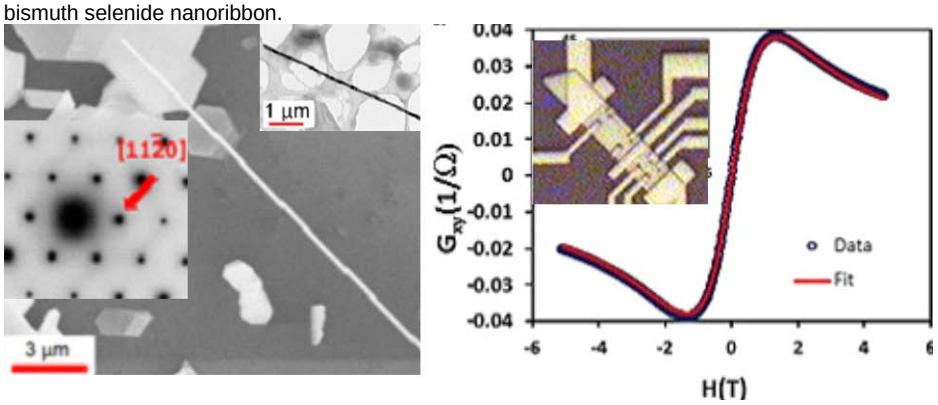
We describe new synthesis techniques and low-temperature transport measurements of nanostructures of high-purity topological insulators bismuth selenide, bismuth telluride and others. Using a catalyst-free, atmospheric pressure vapor-solid growth, with hydrogen as a carrier gas, we obtain a variety of nanostructures: nanowires, ribbons, platelets, and flakes of different sizes and shape. The type of the resulting nanostructures can be controlled using the temperature profile. Materials analysis shows highly ordered structures of bismuth selenide of high purity in all cases, and the nanostructures can be grown on many different substrates. Low-temperature measurements of as-grown nanostructures show strong contributions from the surface states and tunable carrier density in all samples. With appropriate doping, the transport properties of the samples can be tuned from insulating to a superconducting regime.

Acknowledgements.

This work is supported by the National Science Foundation under DMR-1106167 and DGE-1232825 (J. T. M.).

Figure

Figure Caption: Example of the materials analysis of bismuth selenide nanowires and Hall conductance measurements on a bismuth selenide nanoribbon.



Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Surface x-ray structure analysis of prisitine Bi_2Se_3(0001)

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Abstract

We have carried out in situ surface x-ray diffraction (SXRD) experiments to study the atomic structure of the (0001) surface of the topological insulator Bi_2Se_3. Although in general it is well accepted that details of the surface electronic structure as well as potential applications critically depend on the atomic arrangement, only a few studies have been carried out to analyze the surface atomic structure. For the Bi_2Se_3(0001) surface only scanning tunnelling microscopy (STM) was used, which however lacks resolution and is not capable to analyze the subsurface atomic geometry. Moreover, a recent theoretical study has been shown that the subsurface geometry is of utmost importance because expansion of the van der Waals (vdW) gap induces new states in the bulk band gap [3].

In contrast to STM, SXRD is well suited to study the atomic structure of topological insulators due to the finite penetration depth of the x-rays even under external total reflection condition and because the kinematic (single) scattering theory can be applied to analyze the reflection intensities. Our study provides an unprecedented atomically resolved and depth resolved analysis of the near surface structure of pristine Bi_2Se_3(0001).

Experiments were carried out using the ultra-high vacuum (UHV) diffractometer equipped with a microfocus x-ray source (Cu-Kα radiation) and a two-dimensional pixel detector. The bulk samples were grown by the Bridgman method. After transfer into the UHV vessel surface cleaning was carried out in situ either by annealing up to approximately 500°C or by mild sputtering followed by annealing. Low energy electron diffraction (LEED) patterns exhibited sharp and well contrasted spots and Auger electron diffraction did not show any contaminations. Several samples were studied, for all of them we find the same structure parameters within the experimental uncertainties as discussed in the following:

The quantitative analysis of the intensity distribution along four symmetry independent the integer order crystal truncation rods [(10L), (01L), (11L) and (02L)] up to a maximum normal momentum transfer (Qz) of 14 reciprocal lattice units (Qz=3.1 $Å^{-1}$) reveal that the top Se-Bi interlayer spacing (d_{Se-Bi}) is expanded by up to d_{Se-Bi} =10±3% relative to the bulk spacing (1.95 vs. 1.77 Å), while the first vdW gap is contracted by -7%±3% (2.10 vs. 2.25 Å). Ab initio calculations suggest that the unusual expansion of the top layer distance is related to the presence of an extra charge density in the near surface region resulting from the surface state. We also find that an expansion of d_{Se-Bi} in the 10% range and more leads to the appearance of new states within the band gap. Our study sheds new light on the interpretation of the electronic structure based on surface structural relaxations.

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Acknowledgements

The authors acknowledge the help of F. Weiss during the experiments

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Electron scattering on the $BiAg_2$ surface alloy: coherent versus isolated steps

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Abstract

The chiral spin texture of metallic surface states in topological insulators and metals with strong Rashba interaction leads to a unique scattering behavior, characterized by a strong suppression of backscattering. This has been studied by STM in topological semimetals [1] and insulators [2,3], by measuring quantum interference patterns arising from scattering at either disordered or isolated surface defects. In particular in Sb(111) [1], a clear evidence of electron leakage through steps as been observed, which has been attributed to the topological protection against backscattering.

In this work we study the electron transmission through surface steps in the BiAg2 surface alloy. This surface alloy with a strong Rashba interaction hosts helical electrons with a complex energy-dependent spin texture. Despite the strong Rashba splitting of the surface bands, we find no signature of transmission through isolated steps that could derive from a suppression of backscattering. This seems to be related to the fact that the scattering vectors we measure with the interference patterns connect states with opposite average spin, in contrast to what has been observed in topological insulators [2]. Surprisingly, the hard-wall barriers of isolated steps transform into nearly transparent, highly leaking barriers when we add them coherently in a superlattice (see Fig. 1), similar to what we observe in noble metals with negligible spin-orbit coupling [4]. The results highlights the complex scattering scenario in BiAg2, where factors such as defect coherence and the detailed overlapping between wave function and scattering potential may play a more important role than that of the spin-orbit interaction.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Rashba splitting induced by inversion symmetry breaking defects in Bi2Se3 thin films

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Abstract

We investigate the effect of inversion symmetry breaking (ISB) defects on the topologically protected surface states (TPSS) of Bi2Se3 thin films. By first principles calculations, we prove the robustness of the TPSS against the formation of ISB defects, such as stacking faults and twin boundaries. This kind of defects have been observed in real crystals of the Bi2Se3 family grown by van der Waals epitaxy [1] and spark plasma sintering [2]. In addition, we show that the degeneracy of Dirac cones located at opposite surfaces of asymmetric Bi2Se3 thin films is lifted. A Rashba splitting of the bands is caused by the inversion symmetry breaking. The band dispersion and spin texture of the surface states are analyzed and the origin and magnitude of the Rashba splitting is discussed in terms of the slab asymmetry. The Zeeman-type splitting of the TPSS generates a net spin current and provides a new route for spin control with promising applications in spintronics.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

First principles transport calculations on topological surface states scattering

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Abstract

We study the scattering properties of topologically protected states on Sb(111) and Bi_2Se_3(111) surfaces by using the *ab initio* transport code SMEAGOL [1]. We consider different types of defects, such as ad-atoms and extended barriers. In the presence of a strong surface perturbation in the form of a step separating surface terraces we obtain standing-wave states resulting from the superposition of spin-polarized surface states. By Fourier analysis, we identify the underlying two dimensional scattering processes and the spin texture [2]. We find evidence of resonant transmission across the surface barrier at quantum well state energies and evaluate their lifetimes. Our results for the Sb surface are in excellent agreement with experimental findings [3]. We also show that despite the presence of a step edge along a different direction, the surface states exhibit unperturbed transmission around the Fermi energy for states with near to normal incidence.

Finally, we also report our results on transport across Bi(111) bilayer two-dimensional topological insulator, where we find spin-flip backscattering from magnetic ad atoms. These also give rise a long-range real space spin-texture along the edge of bilayer nanoribbons, which may be amenable to measurement using spin-polarized STM techniques [5].

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Acknowledgements

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Figure

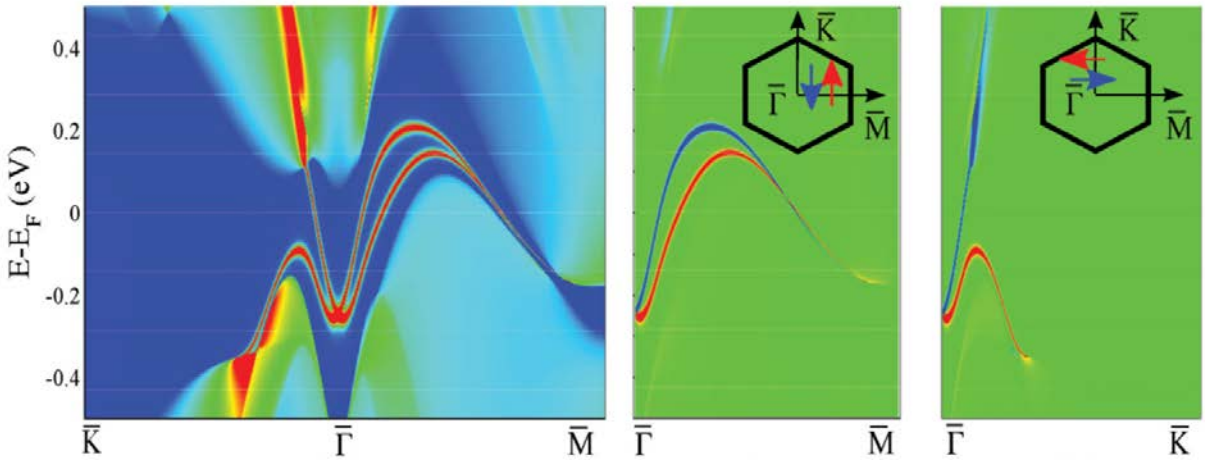

Figure Caption. Simulated ARPES for semi-infinite Sb(111) surface showing the distorted Dirac cone comprising of spin-polarized surface bands. The panels on the right show the spin-resolved ARPES along high symmetry directions. The two surface bands have opposite spin with helical spin texture, as indicated in the insets.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Persistent topological surface state in unoccupied states of Bi_2Te_2Se

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Abstract

Topological surface state with the Dirac-cone energy dispersion and helical spin texture is a manifestation of 3D TIs [1-2]. An interband optical excitation of topological surface states is expected to generate longer-lived spin polarized carriers on the surface by the pulsed laser light [3-4]. To understand the photo-excited spin and charge dynamics, knowledge of empty topological surface state beyond the Dirac point and the unoccupied bulk continuum state is crucial. However, there has so far been a dearth of experimental studies on the unoccupied electronic states of 3D TIs that cannot be accessed by ARPES.

Results of STM / STS study and first principle calculations on the surface of Bi_2Te_2Se in the wide sample bias region will be presented. Clear bias-dependent quasiparticle interference patterns around point defect are observed. In order to obtain the scattering wave vectors, we have performed Fast Fourier transformation (FFT) of the (dI/dV) maps into the momentum-space as described in Figs.1 (a) - (d).

Our results have revealed that the observed scatterings originate from the strongly warped constant energy cuts with substantial out-of-plane spin polarizations of topological surface state. Remarkably, its topological surface state is found to be persistent to more than 1 eV above the Dirac point. This finding opens a new avenue to a deeper understanding of optically excited spin and charge dynamics on the surface of topological insulators.

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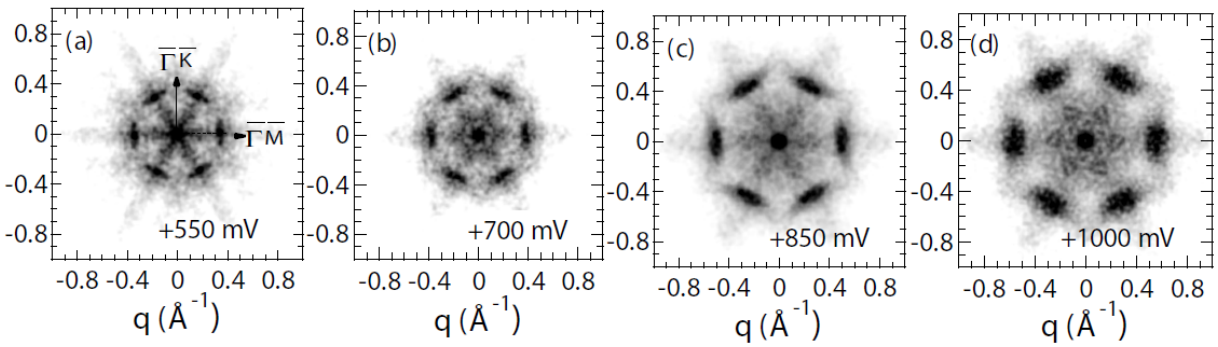
STM and ARPES measurements were performed with the approval of the Proposal Assessing Committee of HSRC (Proposal No.11-B-49, No.10-A-32). This work was financially supported by KAKENHI (Grant No.20340092, 23340105), Grant-in-Aid for Scientific Research (B) of JSPS.

Picture



Picture Caption: (a)-(d) Fast Fourier transformed images of differential conductance map of Bi_2Te_2Se surface acquired at 4.5 K with several sample bias voltages.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Disorder-induced Randomization of Spin Polarization and Interfacially Protected Surface States in Three-dimensional Models of Topological Insulators

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Abstract

We design three-dimensional models of topological insulator thin films, showing a tunability of the odd number of Dirac cones driven by the atomic-scale geometry at the boundaries. A single Dirac cone at the Γ-point can be obtained as well as full suppression of quantum tunneling between Dirac states at geometrically differentiated surfaces. The spin texture of surface states changes from a spin-momentum-locking symmetry to a surface spin randomization upon the introduction of bulk disorder. These findings illustrate the richness of the Dirac physics emerging in thin films of topological insulators and may prove utile for engineering Dirac cones and for quantifying bulk disorder in materials with ultraclean surfaces.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Efficient step-mediated intercalation of silver atoms deposited on the Bi_2Se_3 surface

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Abstract

The evolution of electronic and structural properties of topological insulator surfaces upon deposition of various adsorbates is of significant interest currently [1-5]. Typically, the Dirac state survives upon such an adsorption, however, additional Rashba-split two-dimensional electron gas states arise at the surface, as was shown for Bi_2Se_3 exposed to molecules [1], alkali [2], noble [3, 4] and magnetic [5] metal atoms. Meanwhile, structural investigations of the impurity-deposited Bi_2Se_3 surface revealed partial [2] or almost complete [3, 4] disappearance of adatoms at room and higher temperatures. The authors of these works claimed that majority of the adatoms intercalates below the surface, presumably into the van der Waals gaps of the Bi_2Se_3 crystal, however the mechanism of such an intercalation has not been investigated yet. To study this mechanism we consider the case of the silver atoms deposited on the Bi_2Se_3 surface. Two possible intercalation mechanisms are examined: penetration from the terrace under the step and penetration via interstitials and/or vacancies of the surface quintuple layer block. It is shown that the former mechanism is strongly preferred over the latter one due to significant energy gain appearing at the step. According to performed estimations, the room temperature diffusion length of silver atoms reaches ten microns within a couple of minutes both on the surface and within the van der Waals gap, which essentially exceeds a typical distance between steps. These results shed light on the mechanism of intercalation of metal atoms deposited on the Bi_2Se_3 surface.

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Workshop on NEW TRENDS in TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Coupling topological insulators and magnetic materials: a first-principles study

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Abstract

Combining topological insulators with magnetic materials reveals a rich variety of novel physical phenomena [1,2,3]. Our first-principles calculations address the properties of magnetic impurities on the surface of topological insulators and interfaces between topological insulators and magnetic materials. In particular, we investigate Fe adatoms on the surface of Bi_2Te_3 topological insulator in the context of a recent experimental study [4]. Our calculations performed at the LDA+*U* level of theory reveal preferred adsorption sites, magnetic moments and large magnetic anisotropy energies of Fe adatoms in agreement with experimental results.

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Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Non 100% Spin Polarization in the Ensemble of Photoelectrons from Topological Insulator Thin Films

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Abstract

Spin polarized photoemission spectra from surfaces of Bi_2Te_3 and Sb_2Te_3 thin films [1-2] show up to 45% *in-plane* spin polarization in the Dirac cone near the Fermi level [3-4], which is consistent with the dedicated *ab initio* theoretical results which find spin polarization in the order of 40-50% when averaged over the surface quintuple layer with the exponential depth profile related to the scattering mean free path of the VUV photoelectrons. Furthermore a non-zero *out-of-plane* spin polarization component is found in the Bi_2Te_3 hexagram Fermi surface [3].

We will discuss the spin-orbit entanglement mechanism behind the non-100% spin polarization in topologically protected surface states, and propose possible surface engineering solutions to increase the spin polarization of the Dirac cone in films grown by the MBE. Furthermore we will compare analytical band structure models with the DFT-based slab calculations.

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Figure

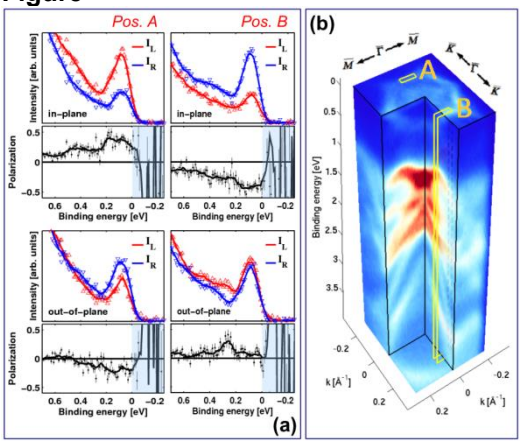

Figure Caption. (a) Spin-polarized data taken near the Fermi on selected k-space locations along the $\overline{\Gamma K}$ direction on the 40 nm Bi_2Te_3 film. The top row indicates the in-plane spin-vector component intensities, whereas the out-of-plane intensities are plotted in the lower rows. **(b)** Experimental three-dimensional band structure of a Bi_2Te_3 thin film over the full valence band region, indicating the k-space volumes A and B which are integrated in the spin-polarized experiment.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

DFT-investigation of a 2D model of the 3D weak topological insulator $Bi_{14}Rh_3I_9$ and study on transition-metal substitutions

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Abstract

We have recently reported the new 3D weak topological insulator $Bi_{14}Rh_3I_9$ [1], a layered compound build of two layer types, in which one, a hexagonal arrangement of $RhBi_8$-cubes, is a 2D TI according to the Kane-Mele model. In contrast to graphene, the gap that is opened in the new compound by spin-orbit interaction, is approximately 240,000 times larger. This new material together with the structurally-related, long-known compound $Bi_{13}Pt_3I_7$ [2] could provide a fruitful playground for research on 2D and weak 3D TIs. Eventually both compounds could become parent structures of a new family of TI materials.

Considering this, there are two issues to tackle. On the one hand, calculations of the edge or surface states should be performed, especially in order to enable direct comparison with physical property measurements. On the other hand, as the two known compounds suggest that a chemical modification is possible, we want to study the impact of transition-element exchange in the intermetallic layer on topological properties.

For a guidepath for further experiments we derived a simple 2D model from the layered structure of $Bi_{14}Rh_3I_9$. This model is essentially the one layer of $RhBi_8$-cubes in the hexagonal arrangement of the original compound (fig. 1 (a)). As DFT based calculations with FPLO (full-potential local-orbital [3]) showed (fig. 2 (b) vs. (c)), the topological properties are the same as for the original compound, which strengthens our idea of $Bi_{14}Rh_3I_9$ as an alternate stacking of a 2D TI (our model) with an insulating spacer.

Consequently, the 2D model opens the possibility to calculate the edge states [4], even in non tight-binding approaches in the FPLO-code. Amongst others, that would allow us to study effects of the different termination of this graphene-like, intermetallic network and could help to interpret physical property measurements. Furthermore, focusing on the second issue, we applied our model for hypothetical compounds with rhodium in the intermetallic layer being exchanged against the other platinum-group elements, namely ruthenium, palladium, osmium, iridium and platinum. Although, $Bi_{13}Pt_3I_7$ is not a TI, the calculations of the electronic structure yielded two other networks which may host a topological non-trivial phase.

Since the synthesis of the parent structure $Bi_{14}Rh_3I_9$ has been very well understood and optimized [5], its protocol can be directly applied for the synthesis of the candidate TI compounds that our theoretical investigation has predicted, thus, enlarging the family of new 3D weak TIs.

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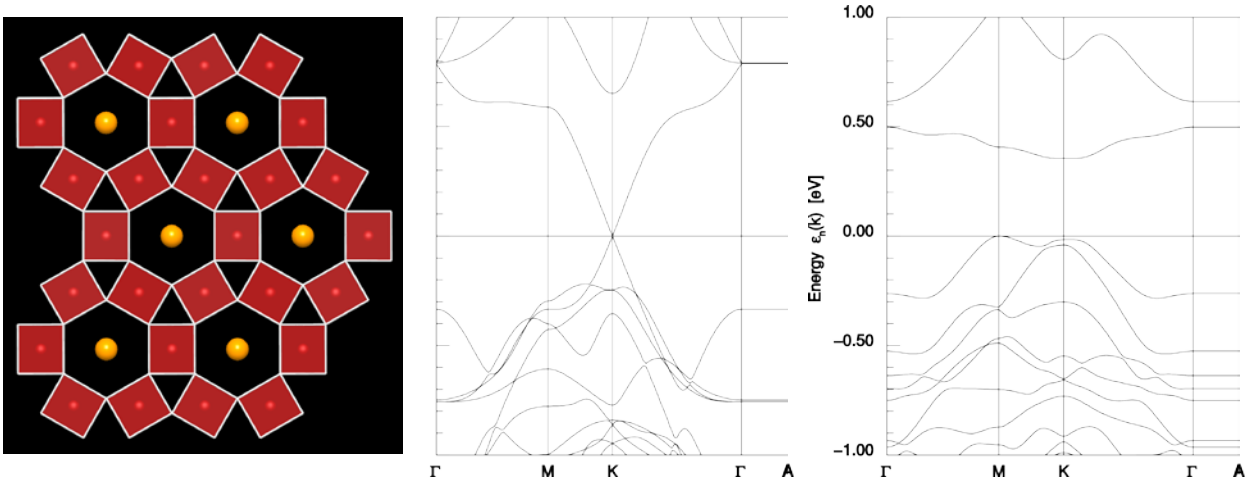
Figure



(a) **(b)** **(c)**

Figure Caption: (a) $RhBi_8$-cubes in the hexagonal arrangement, as found in $Bi_{14}Rh_3I_9$ and in the simple 2D model. (b) scalar and (c) full relativistic band structure calculated with FPLO of the simple 2D model.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols,Girona, Spain - June 3-6, 2013

Bi_2Te_3: A dual topological insulator

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Abstract

We investigate the Z_2 topological insulator Bi_2Te_3 under the influence of magnetic doping or external magnetic field.
In addition to being a Z_2 topological insulator with Z_2 invariants (1;0 0 0) [1], Bi_2Te_3 is also a topological crystalline insulator with mirror Chern number -1. Magnetic doping or external magnetic field breaks the time-reversal symmetry requiered for the Z_2 character, but preserves the mirror-symmetry needed by the topological crystalline character [2], provided the magnetization or the external magnetic field is oriented perpendicular to the mirror plane. The consequence is the shift of the Dirac state off the time-reversal invariant momentum $\bar{\Gamma}$ at the (111) surface, but the crossing of the states at the Dirac point remains protected.
The bulk and surface electronic structure as well as the topological invariants were investigated by means of tight-binding calculations, $\boldsymbol{k}\cdot\boldsymbol{p}$ model and *ab initio* KKR calculations complement and support these results.
Our findings open a new path towards device applications that rely on topological insulators with magnetically controllable topological character.

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Acknowledgements.

This work is supported by the Priority Program 1666 'Topological Insulators' of the DFG.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Electron scattering in the surface alloy

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Abstract

Spin-orbit interaction (SOI) affects the scattering behavior of 2D electrons on surfaces of topological insulators or of metals with strong Rashba interaction. The consequent entanglement between spin and orbit leads to the suppression of backscattering, and can give rise to exotic transport phenomena where pure charge and spin currents can be induced with reduced dissipation [1,2].

Here we use the BiAg2 alloy, which is characterized by the strongest to date Rashba effect [3,4], to study the effect of SOI on scattering. The alloy is formed on the ( ) surface after the deposition of monolayer of Bismuth, which induces a (√ √) reconstruction. The scattering has been studied using Scanning Tunnelling Microscopy (STM) and Spectroscopy (STS). In this way we have studied electron confinement by measuring the interference patterns formed by surface electrons scattered from monoatomic steps. The negligible leakage we observe across the steps indicate a strong confinement effect, comparable to that observed in metals with marginal SOI such as Ag(111) [5]. This is in agreement with the quantized energy levels measured for electrons confined between a pair of steps, comparable to that of infinite quantum wells. Surprisingly, confinement is strong even at energy regions where backscattering is predicted to be prohibited by the spin texture of the electronic states, and where previous STM studies failed to observe interference patterns [6]. Additionally, the effect of the atomic structure of the scatterer has been explored by using two different types of step, where substantial differences have been found both in the scattering strength and asymmetry of the step potential. The latter indicates that, for particular step configurations, scattering is significantly different for electrons going upwards or downwards across the steps.

The results describe a scenario that is far more complex than that of a simple two dimensional free-electron gas in the presence of a strong SOI.

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Figure

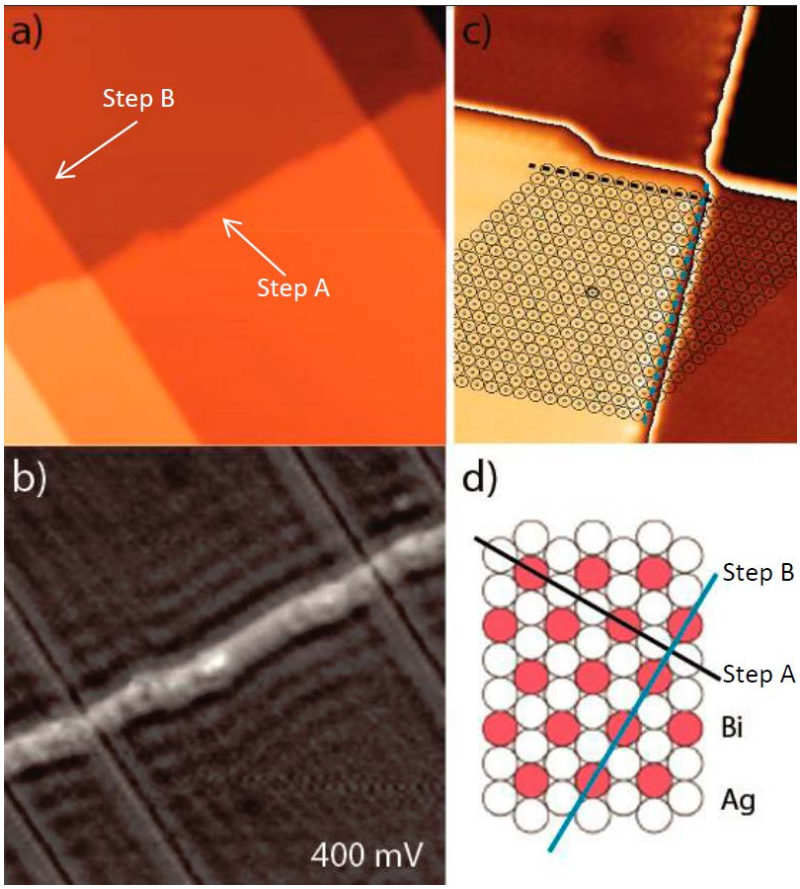

Figure 1: (a) Topographic image of a zone of the sample with different type of monoatomic steps. Image size: 406×406 Å^2. (b) dI/dV-map acquired at $V_{bias} = +0.4$ V. Note that the intensity of the standing wave scattered from the two kinds of step is different. (c) The surface lattice structure resolved in an STM image, where the different termination of each step type can be distinguished. Image size: 164×110 Å^2. (d) Schematics of the lattice of the surface alloy. Solid lines indicate the direction of each step type.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Terahertz Magnetospectroscopy of 2D HgTe Based Topological Insulators

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Abstract

We report on a Terahertz magnetospectroscopy study of a set of five HgTe quantum wells of different thickness, from below to above the critical thickness d_c. In quantizing magnetic fields up to 16 T, both intraband and interband transitions have been observed [1]. In samples with inverted band structures, we confirm the observation of the crossing avoiding of the zero-mode Landau levels [2] at a critical value of the magnetic field (see Fig. 1) [3]. In samples with non-inverted band structures, close to the critical thickness, we report on the square root dependence of the intraband transition energy on the magnetic field, as expected in the single-particle model of massless Dirac fermions. The obtained results are compared with the allowed transition energies calculated using the 8 × 8 Kane model.

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Acknowledgements

This work was supported by CNRS via GDR-I project "Semiconductor sources and detectors of Terahertz frequencies", and by the Languedoc-Roussillon region with the "Terahertz platform" project. The work was also supported by Polish Ministry of Science and Higher Education, via project number N202/103936.

Figure

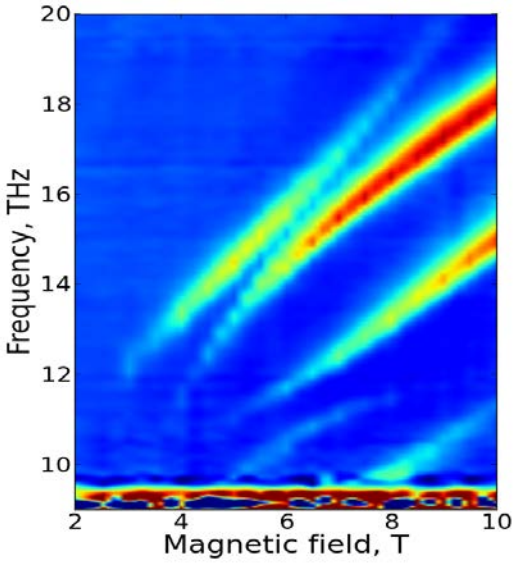

Figure Caption. Histogram of absorption spectra as a function of the applied magnetic field [3], for a HgTe QW with inverted band structure. One can clearly see two anti-crossings at a critical magnetic field of approximately 6 T.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain, June 3-6, 2013

Bi_2Te_3 and $Bi_{1-x}Sb_x$ Nanowires as Topological Insulator Materials: Synthesis and Characterization

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Abstract

Topological insulators are very important materials on the path towards dissipationless electronics and room temperature spintronic applications. A major challenge for 3D topological insulators is the reduction of the large concentration of residual bulk carriers that hide the properties of surface states during electron transport measurements.

We synthesize and investigate topological insulator materials in the form of nanowires with controlled geometry and reduced dimensions. First, etched ion-track templates with cylindrical channels with diameters between 10 and several hundred nanometers, and lengths of tens of micrometer, are fabricated by heavy ion irradiation and selective chemical etching of the ion tracks. Nanowires of the topological insulators Bi_2Te_3, and $Bi_{1-x}Sb_x$ are fabricated in a second step by electrodeposition in the nanochannels of these polymer templates. Their electrochemical growth is investigated and their crystallographic structure and chemical composition is analysed by HRSEM, XRD, TEM, and EDX.[1,2] Electrical transport measurements on topological insulator nanowire field effect transistors will enable us to elucidate the mobility and carrier density of the nanowires as a function of wire diameter and temperature. As the diameter of the wires decreases, e.g. from 500 down to 10 nm, the surface-to-volume ratio increases, and the manifestation of surface states and the electronic and optical properties of the wire can be studied in a systematic manner.

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Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Effect of lattice disorder on the $BiSbTe_2S$ topological surface state.

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Abstract

Band structure engineering by means of varying the chemical composition of the material is a modern trend in the field of topological insulators [1,2]. Another possible way of tuning the electronic structure is the variation of the degree of lattice disorder.

In this contribution we study the stoichiometric $BiSbTe_2S$ compound with substitutions of atoms between Bi and Sb sublattices. First, we calculate the band structure of the ordered $BiSbTe_2S$ using the VASP code. Since the $BiSbTe_2S$ slabs do not have inversion symmetry, we obtain two different Dirac states situated at opposite surfaces of the slab. The respective Dirac points (DP) are considerably separated in energy: one DP is located in the fundamental gap, while the other DP is buried in the valence band.

Further we investigate the Bi-Sb sublattice disorder effects by means of the Korringa-Kohn-Rostoker method and coherent-potential approximation. We study the evolution of the Dirac states under the change of the degree of intermixing of Bi and Sb atoms. In the case of fully disordered Bi-Sb sublattice the inversion symmetry of the slab is restored, and the Dirac states reiding at opposite surfaces are degenerate, with the DP located in the projected energy gap slightly below the valence band maximum.

Thus, we have shown that both the ordered and disordered compounds $BiSbTe_2S$ are topological insulators. Our results provide useful information for the experimental study and band structure engineering of the $BiSbTe_2S$ topological insulator.

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Acknowledgements

This work was supported by the Ministry of Education and Science of Russian Federation (state task No. 2.8575.2013). Calculations were performed on SKIF-Cyberia supercomputer of Tomsk State University.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS

Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Long-range exchange interaction in binary topological insulators

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Abstract

Using a first-principle Green function approach, we study magnetic properties of binary chalcogenides. The estimated magnetic coupling between the impurities is long-range in contrast to what it was believed, and extends beyond a quintuple layer. We discuss two main mechanism of the magnetic interaction in these materials: direct exchange and indirect interaction between magnetic moments via the chalcogen atoms. We estimate the Curie temperature of these systems, which is found in good agreement with the available experimental data, and a way to tune these materials in order to achieve a higher temperature. Our results provide a deep insight into the magnetic interactions in topological insulators and open the way to design new materials for promising applications.

Figure

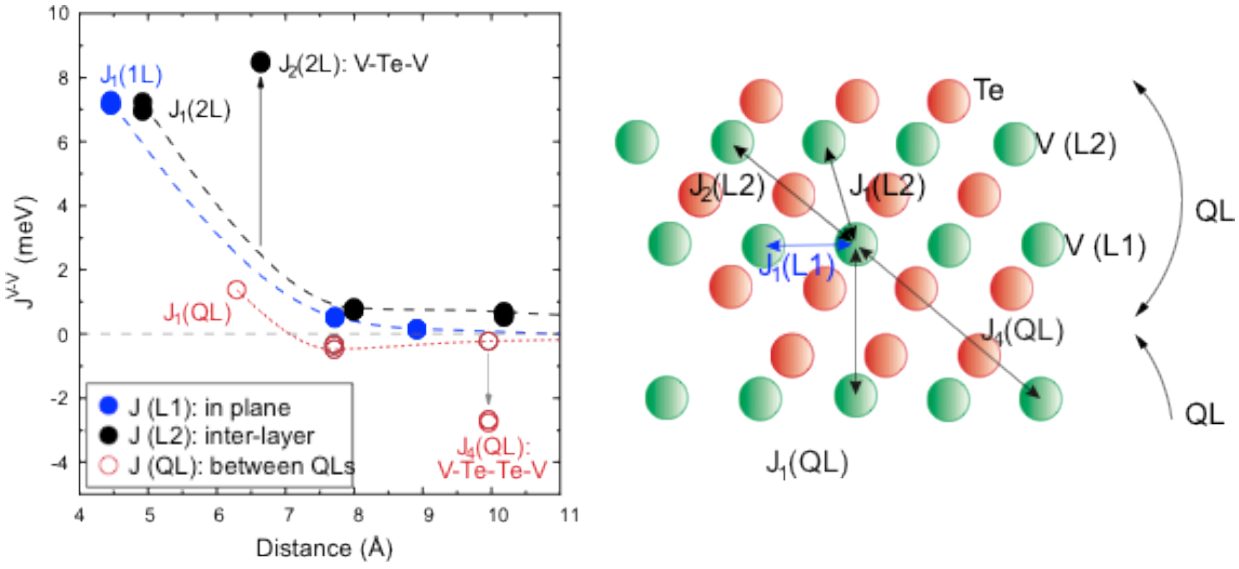

Figure Caption. Exchange constants of $Sb_{1.9}Te_3V_{0.1}$ as a function of the closest neighbors.

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Ambipolar surface quantum Hall effect in the 3D TI strained HgTe

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Abstract

We present magnet-transport experiments in the three-dimensional topological insulator (3D TI) strained HgTe. Using a top-gate, we can tune the carrier concentration of the two-dimensional surface states which enables us to observe an ambipolar surface quantum Hall (SQH) effect of Dirac fermions for the first time.

HgTe is a semimetal and the Dirac-like surface states can only be probed if strain is applied, which leads to a gap opening between the light-hole and the heavy-hole band. Recent experiments on strained HgTe at mK temperatures have shown the SQH effect for electrons thereby proving the 2D nature of this system [1].

We discuss the properties of surface transport in high magnetic fields up to 30 T in terms of the appearance of odd and even integer filling factors within a two-surface model, the geometrical phase, and address the physics of the charge neutrality point. Our experiments demonstrate that high-quality strained 3D HgTe is an ideal material to probe the Dirac-type surface states in 3D TIs.

References

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Acknowledgements

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Figure

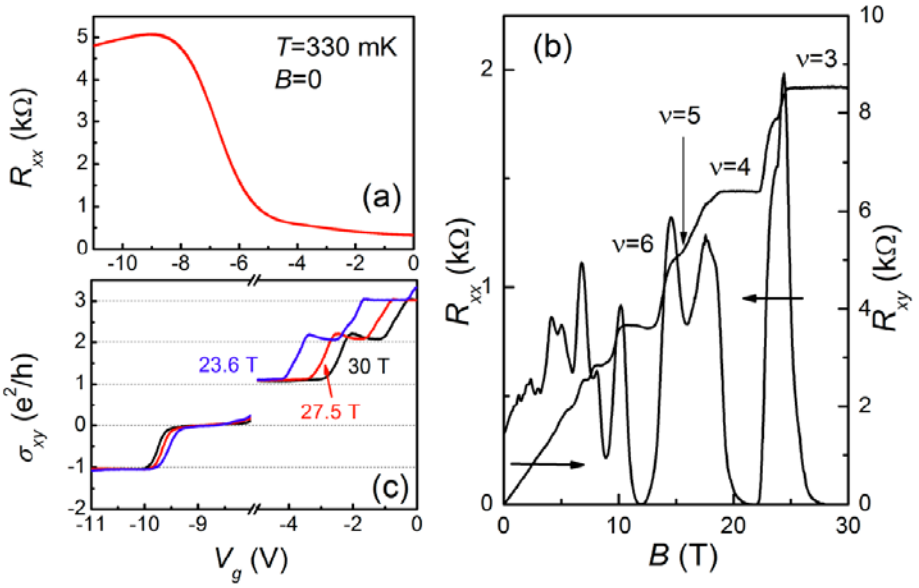

Figure Caption: Magneto-transport measurements in the 3D TI strained HgTe at 330 mK:(a) Gatesweep at *B*=0.(b) *B*-sweep at V_g=0 exhibits SQH effect for electrons where several integer filling factors *v* are observed. (c) Hall conductivity at high magnetic fields shows the transition from electrons (*v*=1) to holes (*v*=-1).

Workshop on NEW TRENDS on TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Synthesis and Quantum Transport Properties of Bi2Se3 Topological Insulator Nanostructures

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Abstract

Bi2Se3 nanocrystals with various morphologies, including nanotower, nanoplate, nanoflake, nanobeam and nanowire, have been synthesized. Well-distinguished Shubnikov-de Haas (SdH) oscillations were observed in Bi2Se3 nanoplates and nanobeams. Careful analysis of the SdH oscillations suggests the existence of Berry's phase p, which confirms the quantum transport of the surface Dirac fermions in both Bi2Se3 nanoplates and nanobeams without intended doping. The observation of the singular quantum transport of the topological surface states implies that the high-quality Bi2Se3 nanostructures have superiorities for investigating the novel physical properties and developing the potential applications.

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Figure

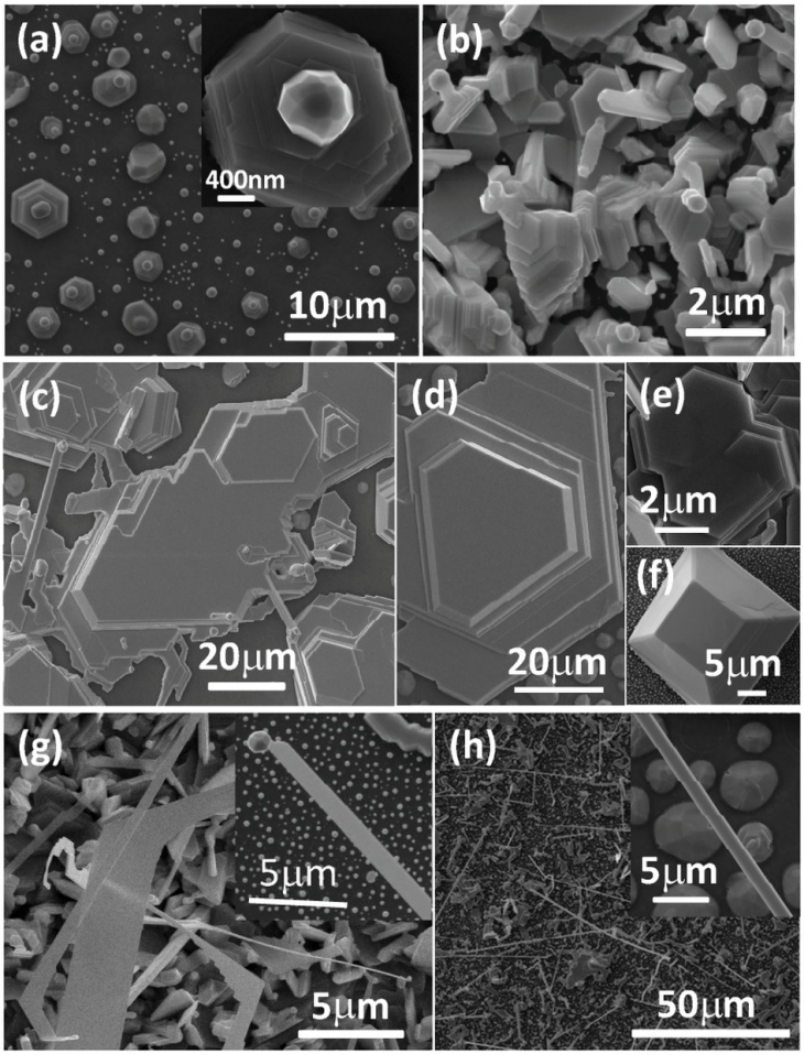

Figure caption 1 (a-h) SEM images of the synthesized Bi_2Se_3 nanostructures with different morphologies by collecting the productions at the places downstream away from the source with different distances.

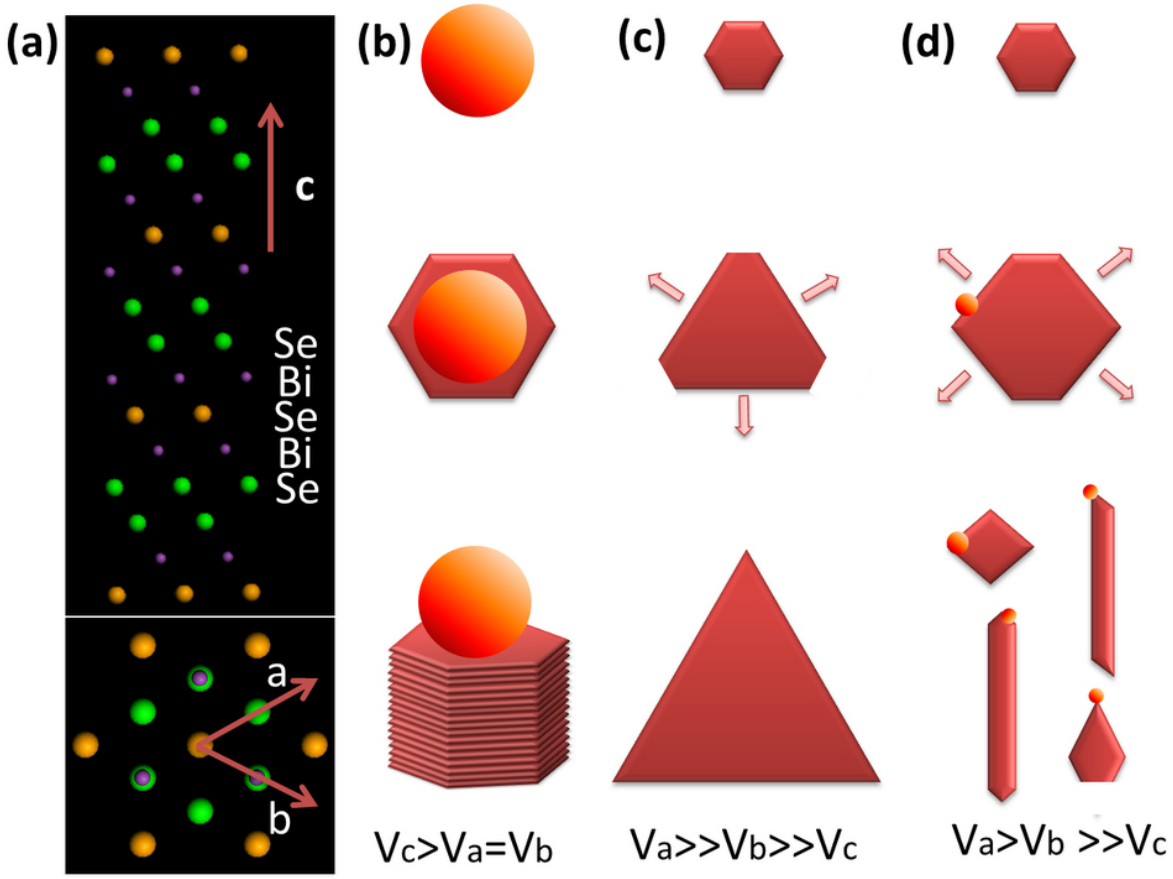

Figure Caption 2 (a) The crystal structures of Bi_2Se_3 from side-view (top panel) and top-view (bottom panel). (b) The vapor-liquid-solid growth along [0001] direction. (c) The dominant growth along [10-10] or [01-10] directions. (d) The growth along [11-20] direction and the formation of quasi-one dimensional structure.

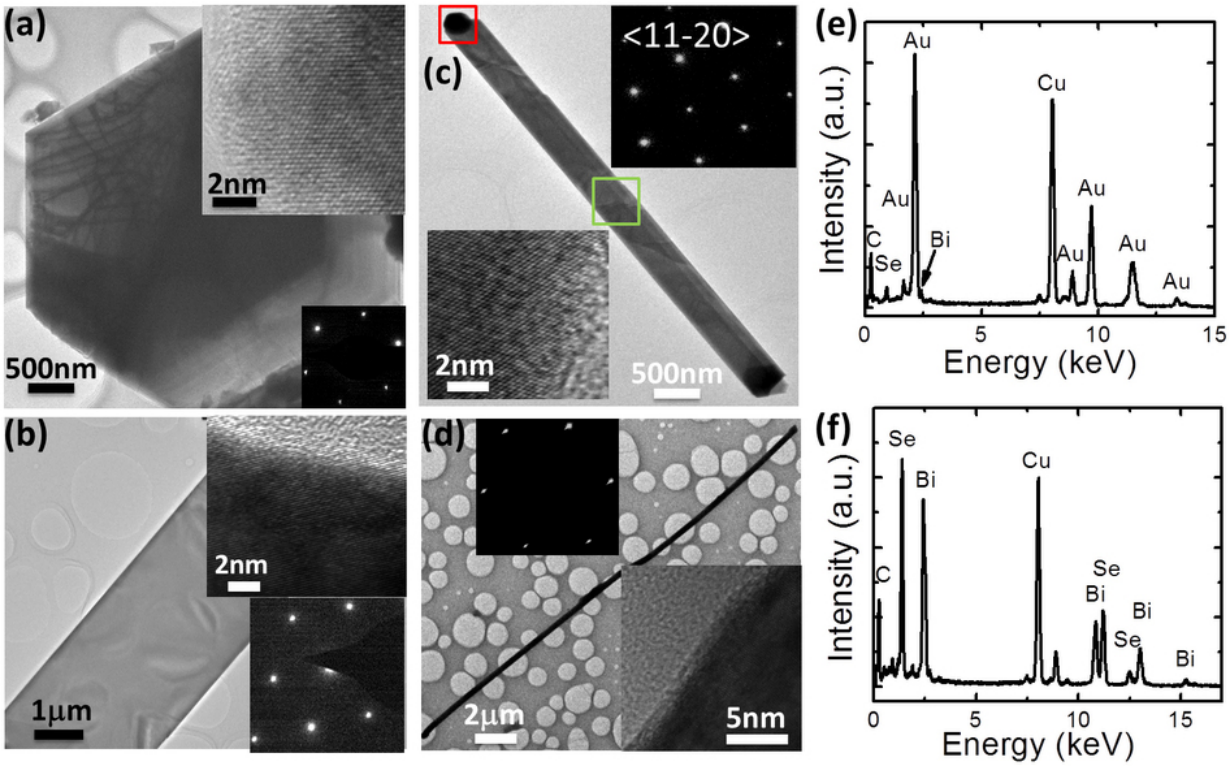

Figure Caption 3 (a-d) TEM images of different Bi2Se3 nanostructures. The insets show the corresponding HRTEM images and selected area electron diffraction patterns. (e, f) EDS spectra collected from the head and body of the Bi2Se3 nanoribbon in panel (c), respectively.

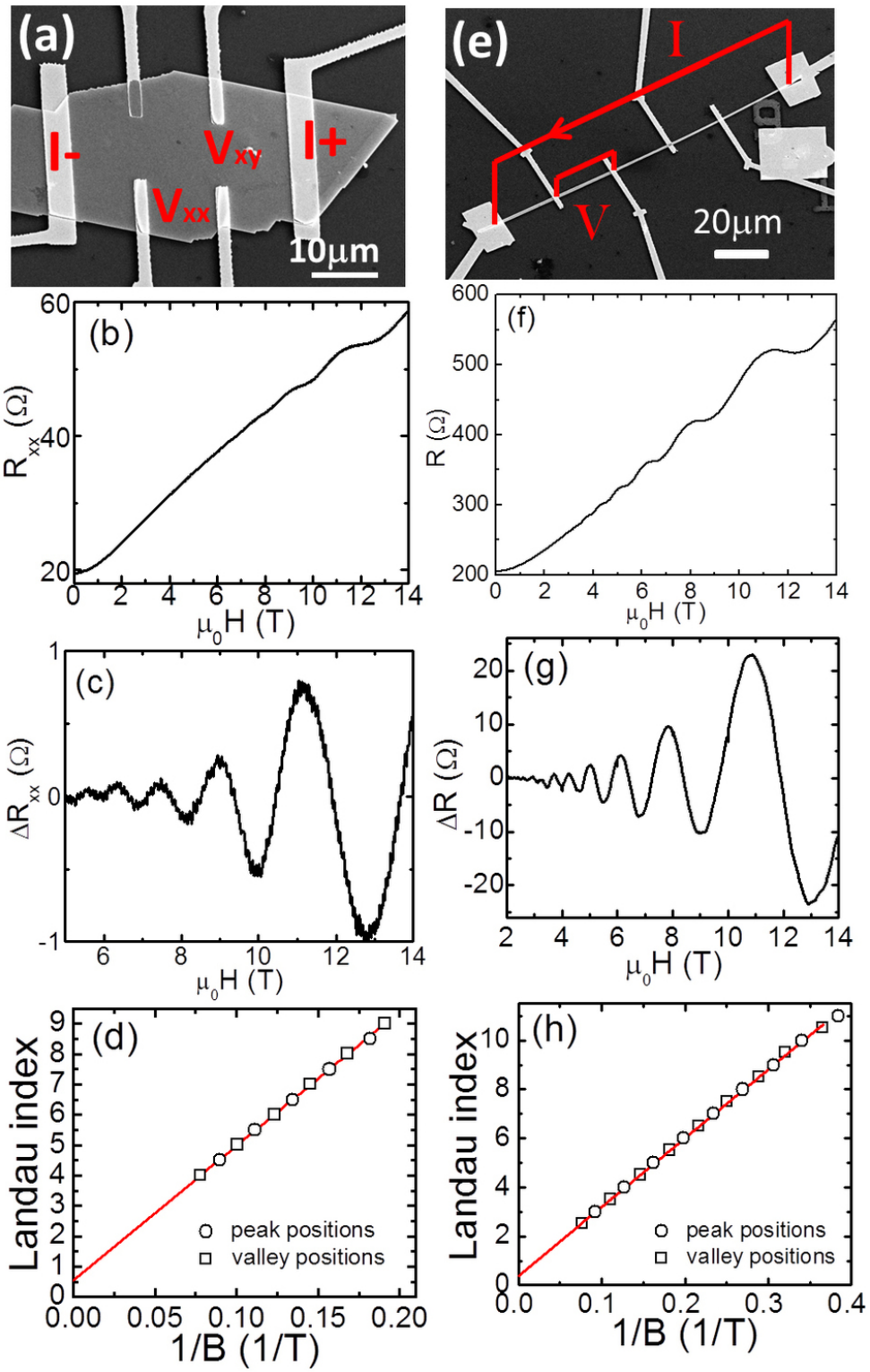

Figure Caption 4 (a-d) are related to the Bi2Se3 nanoplates: (a) the SEM image of an individual Bi2Se3 nanoplate with Hall bar electrodes, (b) the magnetoresistance measured at 1.5 K, (c) the SdH oscillations observed after subtracting the magnetoresistance background, (d) Landau index vs 1/B, the peaks and valleys of the resistance oscillations correspond to N + 1/2 and N and are denoted by the circle and square symbols, respectively; (e-h) are related to the Bi2Se3nanobeams: (e) the SEM image of an individual Bi2Se3 nanobeam with multi-terminal electrodes, (f) the resistance as a function of magnetic field measured at 1.5 K, (g) the resistance oscillations after subtracting the positive magnetoresistance background, (h) Landau index vs 1/B, the peaks and valleys of the resistance oscillations correspond to N and N + 1/2 and are denoted by the circle and square symbols, respectively.

Workshop on NEW TRENDS in TOPOLOGICAL INSULATORS
Sant Feliu de Guíxols, Girona, Spain - June 3-6, 2013

Topological defects in topological insulators: stacking faults in bismuth chalcogenides

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Abstract

Bismuth chalcogenides Bi_2Se_3 and Bi_2Te_3 are currently the most extensively investigated bulk topological insulators. The peculiar layered crystal structure of bismuth chalcogenides implies that the stacking fault defects is an abundant class of non-local imperfections in these materials. In our work we address the atomic structure, formation energies and electronic properties of these topological defects from first principles. In particular, we focus our attention on stacking fault structures that result in mid-gap states of either topologically non-trivial or topologically trivial character. Our results shed light on the properties of highly polycrystalline samples of bismuth chalcogenides such as the thin films grown by means of molecular beam epitaxy. In addition, our work opens new possibilities for engineering the properties of topological insulators.

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