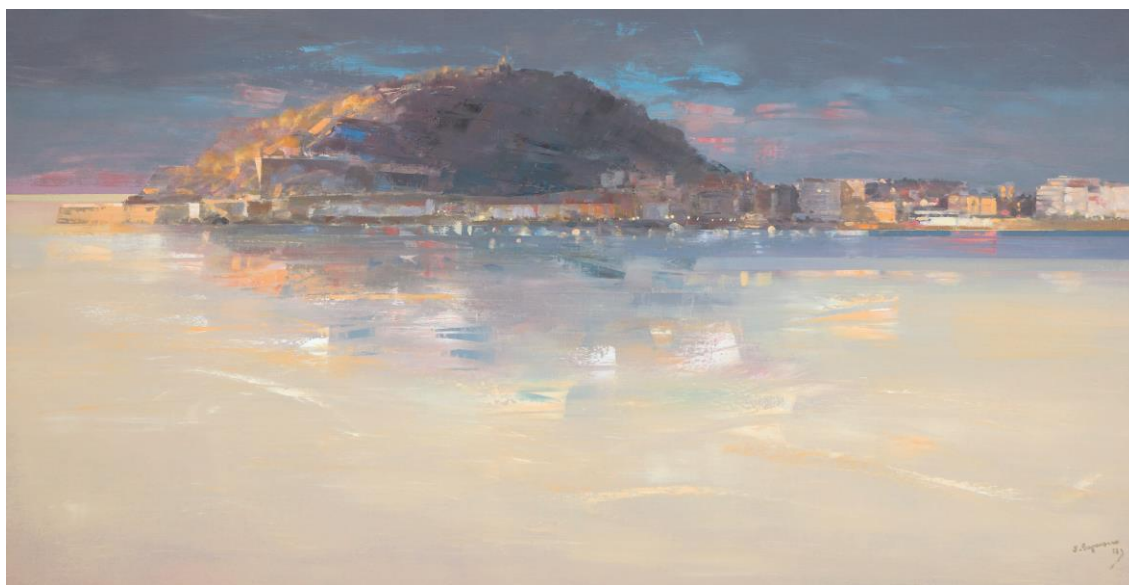


New Trends in Topological Insulators 2015 (NTTI2015)

6-10 July 2015, Donostia-San Sebastian



Scientific committee

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M. Zahid Hasan
Laurens Molenkamp
Sergey Frolov

Organizing committee

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Invited speakers

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Gustav Bihlmayer
Sergey Eremeev
Arthur Ernst
Motohiko Ezawa
Sergey Frolov
Zahid Hasan
Rolph Heid
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Alexey Taskin
Christoph Tegenkamp
Atsushi Tsukazaki
Tonica Valla
Bohm-Jung Yang
Ali Yazdani
Oleg Yazyev

MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
6.07	7.07	8.07	9.07	10.07
8:30 REGISTRATION 9.50 WELCOME				
(10:00) Hasan 40' +Louvet	Molenkamp 40' Yazdani 40' +Pientka+Ojanen	Moodera 40' Ezawa 40' Kimura 40'	Tegenkamp 40' +Basov+Ortmann +Bercioux+Eguchi	Bihlmayer 40' +Vozmediano+Fruchart +Nogueira+Aguilera
coffee				
Schnyder 40' Bernevig 40' +Soluyanov +de Vries	Frolov 30' Sochnikov 30' +Galletti+Kanigel +Reyes-Calvo	Tsukazaki 30' Ernst 30' Pfnür 30' Valla 30'	Sobota 30' Heid 30' Rader 30' Yazyev 30'	Meyerheim 30' +Cerdá+Muñoz +Ngabonziza CLOSING
lunch				
Yang 30' +Shikin+Schäfer +Krieg	Tanaka 30' +Hutasoit+Dufouleur +Essert+Pan (until 16:50)	Taskin 30' +Ferreiros +Souza +Zubizarreta	Politano 30' +Kastl+Plank +Ganichev	15:00-16:30 DEPARTURE
coffee				
Eremeev 30' +Benia+Volobuev+ +Akiyama	POSTER SESSION (+snacks/drinks)	Soljacic 40' +Quelle+Autore (until 18:20)	FREE	17:00-18:30
	17:00-20:00	Conference dinner 20:30	TIME	

Program

Monday, July 06th. Electronic structure

8:30-09:50	Registration	
9:50-10:00	Welcome	
Chairman A. Yazdani		
10.00-10:40	M. Z. Hasan	“Weyl Semimetals, Fermi arcs and 2D Topological Superconductors”
10.40-11.00	T. Louvet	“Minimal Conductivity, Topological Berry Winding and Duality in Three-Band Semimetals”
11.00-11.30	Coffee break	
Chairman A. Kimura		
11.30-12.10	A. P. Schnyder	“Classification of topological quantum matter with reflection symmetries”
12.10-12.50	B. A. Bernevig	“Prediction of Weyl Semimetal in TaAs”
12.50-13.10	A. A. Soluyanov	“Topological invariants made simple: application to new type of topological semimetals”
13.10-13.30	E. K. de Vries	“Anomalous features in electrical probing of spin-momentum locking in Bi ₂ Se ₃ ”
13.30-15.00	Lunch	
Chairman A. Politano		
15.00-15.30	B. J. Yang	“Classification of three dimensional Dirac semimetals”
15.30-15.50	A.M. Shikin	“Dirac cone spin structure of topological insulators for generation of spin currents under circular dichroism photoexcitation”
15.50-16.10	J. Schäfer	“Tunable Electronic Structure and Dirac Cone Warping in the Elemental Topological Insulator α -Sn”
16.10-16.30	J. Krieg	“Characterization of the Electronic Structure along Single Bi ₂ Te ₃ Nanowires by nano-Angle-Resolved Photoemission Spectroscopy”
16.30-17.00	Coffee break	
Chairman R. Heid		
17.00-17.30	S. V. Eremeev	“Non-Dirac topological surface states in (SnTe) _{n>1} (Bi ₂ Te ₃) _{m=1} ”
17.30-17.50	H. M. Benia	“Dirac States On The Noncentrosymmetric BiPd Surface”
17.50-18.10	V. Volobuev	“Giant Rashba Splitting in (111) Pb _{1-x} Sn _x Te Topological Crystalline Insulator Epilayers Induced and Tuned by Bi Doping”
18.10-18.30	R. Akiyama	“Two-dimensional weak antilocalization in topological crystalline insulator SnTe thin films”

Tuesday, July 07th. Superconductivity and Majorana fermions. Transport

Chairman O. Rader		
9.00-9:40	L. W. Molenkamp	“HgTe as a Topological Insulator”
9.40-10:20	A. Yazdani	“Spotting the elusive Majorana under the microscope”
10.20-10:40	F. Pientka	“Strong localization of Majorana end states in chains of magnetic adatoms”
10.40-11:00	T. Ojanen	“Exotic topological superconductivity and high Chern numbers in lattices of magnetic adatoms on a superconductor”
11.00-11.30	Coffee break	
Chairman D. N. Basov		
11.30-12.00	S. Frolov	“Search for additional signatures of Majorana fermions in semiconductor nanowires coupled to superconductors”
12.00-12.30	I. Sochnikov	“Non-contact current-phase measurements of topological weak links with scanning SQUID”
12.30-12.50	L. Galletti	“Unconventional Current-Phase Relation in Coplanar Proximity Devices”
12.50-13.10	A. Kanigel	“The electronic structure of superconducting Cu intercalated Bi ₂ Se ₃ ”
13.10-13.30	M. Reyes Calvo	“Lateral heterojunctions on inverted HgTe quantum wells”
13.30-15.00	Lunch	
Chairman T. Valla		
15.00-15.30	Y. Tanaka	“Crossed surface flat bands of Weyl semimetal superconductors”
15.30-15.50	J. A. Hutasoit	Topologically protected charge transfer along the edge of a chiral p-wave superconductor
15.50-16.10	J. Dufouleur	“Pseudo-ballistic Transport in 3D Topological Insulator Quantum Wires”
16.10-16.30	S. Essert	“Two-Dimensional Topological Insulator Edge State Backscattering by Dephasing”
16.30-16.50	Y. Pan	“Low carrier concentration crystals of the topological insulator Bi _{2-x} Sb _x Te _{3-y} Se _y : a magnetotransport study”
17.00-20.00	Poster session (drinks/snacks)	

Wednesday, July 08th. Quantum Hall effects. Magnetism. Photonics. Plasmonics

Chairman A. P. Schnyder		
9.00-9:40	J. S. Moodera	“Ferromagnetic topological insulator and quantum transport”
9.40-10:20	M. Ezawa	“Topological Insulators with Magnetic Texture”
10.20-11:00	A. Kimura	“Surface Dirac fermion dynamics of non-magnetic and magnetic topological insulators”
11.00-11.30	Coffee break	

Chairman G. Bihlmayer		
11.30-12.00	A. Tsukazaki	“Quantized Hall effects in topological insulator field-effect transistor”
12.00-12.30	A. Ernst	“Magnetism and topological insulators”
12.30-13.00	H. Pfnür	“Magnetic impurities and magnetotransport in ultrathin crystalline Bi films”
13.00-13.30	T. Valla	“Interactions of Topological (Crystalline) Insulators with Superconductivity and Magnetism”
13.30-15.00	Lunch	

Chairman S. V. Eremeev		
15.00-15.30	A. A. Taskin	“Anisotropic Magneto-Resistance and Planar Hall Effect in Dual-Gated Topological Insulator Thin Films”
15.30-15.50	Y. Ferreiros	“Domain Walls in Junctions of Thin Film Magnets and 3D Topological Insulators”
15.50-16.10	I. Souza	“Chiral degeneracies and Fermi-surface Chern numbers in bcc Fe”
16.10-16.30	X. Zubizarreta	“ <i>Ab initio</i> Study Of Electronic And Magnetic Properties Of Fe-doped Topological Insulators”
16.30-17.00	Coffee break	

Chairman A. Ernst		
17.00-17.40	M. Soljacic	“Topological phenomena in photonics”
17.40-18.00	A. Quelle	“Artificial graphene under the spotlight: a realization of the Bernevig-Hughes-Zhang model”
18.00-18.20	M. Autore	“Dirac plasmonics of Topological Insulators”
20:30	Conference dinner	

Thursday, July 09th. Transport. Plasmons. Phonons

Chairman S. Frolov		
9:00-9:40	C. Tegenkamp	“Surface transport on bulk and thin film topological insulators”
9.40-10:00	D. N. Basov	“Sum rule constraints on the surface state conductance of topological insulators”
10.00-10:20	F. Ortmann	“Mesoscopic Charge Transport Simulations for Topological Insulators”
10.20-10:40	D. Bercioux	“Driven Topological Insulator Quantum Dot: A spin-particle source (SPPS)”
10.40-11:00	G. Eguchi	“Transport Properties of the Ideal Surface Dirac Cone in the Topological Insulator $\text{Tl}_{1-x}\text{Bi}_{1+x}\text{Se}_2$ ”
11.00-11.30	Coffee break	

Chairman J. S. Moodera

11.30-12.00	J. A. Sobota	“Ultrafast Electron and Lattice Dynamics of a Topological Insulator”
12.00-12.30	R. Heid	“Electron-Phonon Interaction in Surface States of Topological Insulators from First Principles”
12.30-13.00	O. Rader	“Samarium hexaboride: a trivial surface conductor”
13.00-13.30	O. V. Yazyev	“High-throughput search of novel topological materials”
13.30-15.00	Lunch	

Chairman H. L. Meyerheim

15.00-15.30	A. Politano	“Plasmons in topological insulators: from basic research to technological application in THz photodetection”
15.30-15.50	C. Kastl	“Optoelectronic control and characterization of surface state transport in bismuth-based topological insulators”
15.50-16.10	H. Plank	“Terahertz Radiation Induced Trigonal Photocurrents in $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ Three Dimensional Topological Insulators”
16.10-16.30	S. D. Ganichev	“Cyclotron Resonance Induced Photocurrents in HgTe 3D TIs”
16.30-...	Free time	

Friday, July 10th. Magnetism, electronic and crystal structure

Chairman O. V. Yazyev		
9:00-9:40	G. Bihlmayer	“Prediction and design of quantum spin Hall and quantum anomalous Hall phases from first principles”
9.40-10:00	M. A. H. Vozmediano	“Hall viscosity from elastic gauge fields in Weyl crystals”
10.00-10:20	M. Fruchart	“Topological Index For Periodically Driven Time-Reversal Invariant 2D Systems”
10.20-10:40	F. S. Nogueira	“Field Theory of Proximity-Induced Magnetism in Topological Insulators”
10.40-11:00	I. Aguilera	“Relativistic GW Calculations for Topological Insulators: Quasiparticle Effects on the Bulk and Surface States”
11.00-11.30	Coffee break	

Chairman J. Sobota

11.30-12.00	H. L. Meyerheim	“Atomic and electronic structure of the pristine and adsorbate covered Bi ₂ Se ₃ (0001) surface”
12.00-12.20	J.I. Cerdá	“Tunable Dirac electron and hole self-doping of topological insulators induced by stacking defects”
12.20-12.40	F. Muñoz	“Topological Crystalline Insulator in a new Bi semiconducting phase”
12.40-13.00	P. Ngabonziza	“In-situ Spectroscopy of Intrinsic Bi ₂ Te ₃ Topological Insulator Thin Films And Impact of Extrinsic Defects”
13.00-13.30	Closing	
13.30-15.00	Lunch	
15.00	Departure	

Poster session

P1	V. N. Men'shov, "Confined Electron States in Heterostructures based on 3D Topological Insulators (towards a better understanding of the QSHE) "
P2	J. Kellner, "Tuning the Fermi energy to the Dirac point in the ternary topological insulator $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ "
P3	M. Marciani, "Chaotic Quantum Dots with Tunnel barrier – Scattering from a Majorana bound state"
P4	P. Leubner, "The Effect Of Strain On The Two-Dimensional Topological Insulator HgTe "
P5	I. I. Klimovskikh , "Influence of the surface reorganization on the spin electronic structure of the Dirac cone of topological insulators"
P6	K. Le Calvez, "Missing Shapiro Step in Bi_2Se_3 Josephson Junction"
P7	P. Rüssmann, "First-principles approach to microscopic understanding of quasiparticle interference on the strong topological insulator Bi_2Te_3 "
P8	C. Niu, "Topological Crystalline Insulator and Quantum Anomalous Hall States in IV-VI based Monolayers and their Quantum Wells"
P9	C. Pauly, "Probing the electronic and structural properties of the first weak 3D topological insulator $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ by scanning tunnelling microscopy"
P10	S.-Y. Xu, "Experimental Discovery of the Weyl semimetal state in TaAs"
P11	G. Knebl, "Fabrication and characterization of GaSb/InAs double quantum wells for tunable topological insulator devices"
P12	L. Cornils, "A combined XMCD, ARPES and STM study of 3d adatoms on the topological insulator Bi_2Te_3 "
P13	M. V. Filianina, "Modification of Atomic, Electronic And Spin Structure of Pb-based Quaternary Topological Insulator With Various Stoichiometry"
P14	M. Papaj, "Nanoconstrictions in Quantum Spin Hall Effect Materials"
P15	J. Reimann, "Ultrafast Electron Dynamics of the Topological Insulator Sb_2Te_3 Studied with Tunable Pump Photon Energies"
P16	J. Wiedenmann, " 4π contribution to the Josephson supercurrent in a HgTe based topological Josephson junction"
P17	I. Rusinov, "Pressure Induced Topological And Crystal Phase Transitions In BiTeX ($\text{X}=\text{I}, \text{Br}, \text{Cl}$)"
P18	T. V. Menshchikova, "Tuning the Dirac Point Position in Bi_2Te_3 "
P19	M. Bianchi, "Strongly anisotropic spin-orbit splitting in a two-dimensional electron gas"
P20	A. Isaeva, "Search for new topological insulators among halogen-containing Ti_5Te_3 structural derivatives"
P21	D. Gosálbez-Martínez, "Ferromagnetic iron as a topological metal "
P22	A. Akrap, "Magneto-optical and magneto-transport signatures of giant Rashba splitting in BiTeBr and BiTeCl "
P23	T. Bathon, "Systematics Of Hybrid Organic-Topological Insulator Heterostructures"

P24	M. Fanciulli, “Spin-resolved ARPES as a probe for the phase of the photoelectron wavefunctions”
P25	T. Schumann, “Laser induced DC photocurrents in a Topological Insulator thin film in the transition from p- to n-doping”
P26	H. Aramberri, “Oscillatory exchange coupling and massive Dirac state spin texture in Cr thin films coupled to Bi ₂ Se ₃ surfaces”
P27	I.V. Silkin, “Ultrathin Tetradymite-like 3D Topological Insulator”
P28	P. S. Mandal, “Observation of gapped surface states in the topological regime of the quantum-phase transition in Bi-doped Pb-Sn-Se (111) epitaxial films ”
P29	F. Teppe, “Terahertz Spectroscopy of 2D and 3D Topological Phase Transition”
P30	A. G. Ryabishchenkova, “ <i>Ab initio</i> study of adsorption and diffusion of the I-, IIA- and IIIA- group adatoms on the surface of topological insulator Bi ₂ Se ₃ ”
P31	T. Khouri, “High temperature Quantum Hall Effect in HgTe/HgCdTe quantum wells with a bulk band gap”
P32	B. Rasche, “Tuning the first weak 3D-TI Bi ₁₄ Rh ₃ I ₉ for transport measurements”
P33	A. Inhofer, “High Frequency Capacitance Measurements In Three-Dimensional Topological Insulators”
P34	P. Hlawenka, “ARPES Characterization of the Surface Modified Kondo Insulator SmB ₆ ”
P35	J. Zaldivar, “Searching for Majorana Modes in Mo-S ₂ -Superconductor Heterostructures”
P36	I. A. Nechaev, “Quasiparticle spectrum and bulk plasmons dispersion in the topological insulator Sb ₂ Te ₃ ”
P37	R. Wallauer, “Progress on Time-of-Flight Momentum Microscopy Towards μm and meV Photoelectron Spectroscopy”
P38	H. Ebisu, “ Odd-frequency Pairing In Topological Superconductivity In A One Dimensional Magnetic Chain”
P39	J. Sánchez-Barriga, “Ultrafast spin polarization control of Dirac Fermions in topological insulators”
P40	K. Song, “Signatures of Twin Grain Boundary Formation in the Band Structure of Bi ₂ Se ₃ Topological Insulator”

Weyl Semimetals, Fermi arcs and 2D Topological Superconductors

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Topological materials host Dirac, Majorana and Weyl fermions on their boundaries as forms of topology change excitations [Rev. of Mod.Phys. 82, 3045 (2010)]. I report our recent results on 2D topological superconductors (TSC) as vortex Majorana platforms (Nature Physics 2014), gapless topological semimetals with Fermi arcs (Science 2015) and topological Weyl semimetals as fractional Fermi arc platforms [Nature, submitted]. These new phases of matter and novel excitation modes collectively reveal the emergence of a topological revolution in condensed matter physics.

Minimal Conductivity, Topological Berry Winding and Duality in Three-Band Semimetals

T. Louvet, P. Delplace, A. A. Fedorenko, D. Carpentier

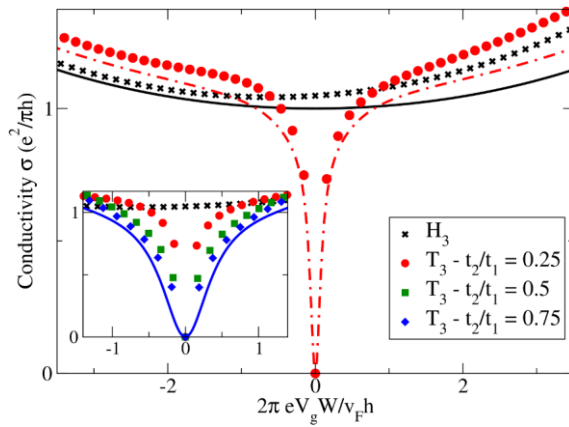
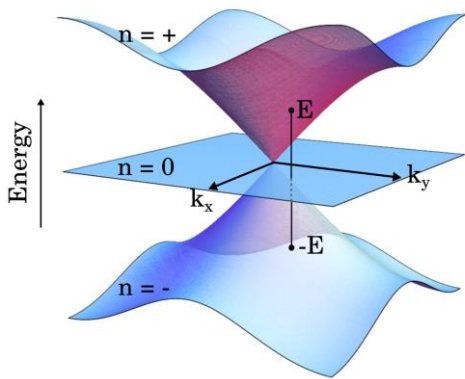
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The physics of massless relativistic quantum particles has recently arisen in the electronic properties of solids following the discovery of graphene. Around the accidental crossing of two energy bands, the electronic excitations are described by a Weyl equation initially derived for ultra-relativistic particles. Similar three and four band semimetals have recently been discovered in two and three dimensions [1,2].

Among the remarkable features of graphene are the characterization of the band crossings by a topological Berry winding, leading to an anomalous quantum Hall effect [3], and a finite minimal conductivity at the band crossing while the electronic density vanishes [3,4]. We show that these two properties are intimately related [5]: this result not only sheds a new light on the origin of minimal conductivity in semimetals, but, most importantly, it paves the way to a direct measure of the topological nature of a semimetal.

By considering three band semimetals with a flat band in two dimensions, we find that only few of them support a topological Berry phase. The same semimetals are the only ones displaying a non vanishing minimal conductivity at the band crossing. The existence of both a minimal conductivity and a topological robustness is related not to the relativistic nature of the electronic excitations, but to phase properties of the electronic wave functions. We show that these remarkable signatures originate from properties of the underlying lattice, which are encoded not by a symmetry of their Bloch Hamiltonian, but by a duality. Relevance of our results to three-dimensional systems will also be discussed.



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CLASSIFICATION OF TOPOLOGICAL QUANTUM MATTER WITH REFLECTION SYMMETRIES

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Topological materials have in recent years become a subject of intense research due to fundamental considerations as well as potential use for technical applications in device fabrication and quantum information. One of the hallmarks of topological materials is the existence of protected exotic zero-energy surface states, which arise as a consequence of a nontrivial topology of the bulk wave functions. In this talk, starting from the ten-fold classification of topological insulators and superconductors, I will survey recent developments, with a particular emphasis on the topological classifications of fully gapped and gapless materials in terms of crystal reflection symmetries [1]. As concrete examples, I discuss the Dirac materials Ca_3PbO and Sr_3PbO [2,3] and show that these antiperovskites are reflection-symmetry-protected topological insulators. The Dirac surface states of these materials are protected by a non-zero mirror Chern number, which can take on only even values. As an example of a reflection-symmetry-protected topological semimetal, I will present results about the recently discovered compound Ca_3P_2 [4] and demonstrate that this system exhibits surface states which are almost dispersionless. If time permits, I will also discuss some results about the topological properties of noncentrosymmetric superconductors [5-8]. In particular, I will show how reflection symmetry gives rise to protected topological arc surface states in these superconductors [9].

References

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Prediction of Weyl Semimetal in TaAs

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Weyl Semimetals are a new phase of matter whereby the metallic behavior is protected by the Fermi Surface topology. I will discuss our recent prediction of a Weyl semimetal phase in TaAs - which was subsequently discovered experimentally - and then present two new materials where we predict Weyl physics will occur. One of these materials hosts a completely new, previously unknown type of Weyl semimetal. This new Weyl type exhibits a different type of chiral anomaly, and appears in high-symmetry planes in materials with Mirror and C_2 symmetries. We then present a general route towards searching for Weyl semimetals based on the material symmetries, and classify all the possible types of Weyls based on the theory of quadric surfaces.

Topological invariants made simple: application to new type of topological semimetals

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In recent years a plethora of different topologies of band structures was found, going beyond the original idea of time-reversal symmetric topological insulators. Examples include but are not limited to crystalline topological insulators (TCI) and topological semimetals (TS). Different topological invariants describe different band topologies, and a generic algorithm is required for finding materials candidates (including TCI and TS). We present a generic algorithm, as well as the associated software package, that operate as a postprocessing tool for a variety of first-principles packages and obtains topological invariants from *ab initio* wavefunctions.

We further illustrate the power of our approach with real material examples, specifically semimetals, where non-trivial topology is especially hard to reveal. Our major finding is a new type of topological semimetals. In particular, a new type of Weyl points exists in these materials and, as a one of the consequences, one can induce a variety of topological Lifshits transitions by strains and doping. A detailed study of one such material is presented.

References

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Anomalous features in electrical probing of spin-momentum locking in Bi_2Se_3

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Topological insulators (TIs) provide a new platform for spintronic applications due to the unique spin texture of the surface states and their suppressed backscattering, originating from the time-reversal symmetry intrinsic to these materials [1-2]. The spin-momentum locking of the surface states is well investigated through ARPES measurements where 100% spin polarization is reported. More recently, first experiments on electrical detection of this spin texture have been reported following the proposed three-terminal potentiometric measurement discussed in Ref. 3. Using ferromagnetic (FM) contacts, spin accumulation can be measured by probing the potential directly underneath the contact [4-5]. The observed hysteresis upon inverting the ferromagnet's magnetization is claimed to originate from the spin imbalance in the surface states.

In this work, we report on our observations of electrical probing of spin momentum locking using well-characterized thin films of Bi_2Se_3 combined with Co/TiO_2 ferromagnetic detectors. Large area homogeneous thin films of Bi_2Se_3 allow for the design of ferromagnetic detector electrodes along different orientations in the entire film surface and proves to be important in the investigation and understanding of the origin of spin-momentum locking of the surface states in such materials. Using a Hall bar patterned device and by changing the direction of the applied current in the TI channel and the magnetization of the ferromagnetic detectors relative to the applied current we obtain similar hysteresis loops as reported in Ref. 4 and 5. However, a careful analysis of the spin voltage obtained for biases both along and perpendicular to the TI channel shows anomalous features which can be easily mistaken as originating from a spin imbalance of the surface states. In this work, we will discuss these important findings and argue that the observed anomalous features in the spin voltage of the TI channel necessitates an alternative explanation based on a detailed analysis of the directionality of the applied bias, temperature dependence, dependence on the contact resistance and specifically on the influence of the effective magnetic field originating at the FM detectors.

References

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Classification of three dimensional Dirac semimetals

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A three-dimensional (3D) Dirac semimetal (SM) is the 3D analogue of graphene having linear energy dispersion around Fermi points. Owing to the nontrivial topology of electronic wave functions, the 3D Dirac SM shows nontrivial physical properties and hosts various exotic quantum states such as Weyl SMs and topological insulators under proper external conditions. There are several kinds of Dirac SMs proposed theoretically and partly confirmed experimentally, but its unified picture is still missing. In this talk, we propose a general framework to classify stable 3D Dirac SMs in systems having the time-reversal, inversion and uniaxial rotational symmetries. We show that there are two distinct classes of 3D Dirac SMs. In one class, the Dirac SM possesses a single Dirac point at a time-reversal invariant momentum on the rotation axis. Whereas the other class of Dirac SMs has a pair of Dirac points created by band inversion, and carries a quantized topological invariant. Moreover, we show that a quantized topological charge can be assigned to each Dirac point which ensures the stability of 3D Dirac semimetals.

Dirac cone spin structure of topological insulators for generation of spin currents under circular dichroism photoexcitation

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Topological insulators (TIs) characterized by metallic-like topologically-protected surface states (TSS) with the helical Dirac cone spin structure arranged in the bulk energy gap are considered now as ones of the best candidates for constructing spintronic devices with effective formation of spin currents and their controlled manipulation. In this our work we will analyze a relation of the features of the electronic and spin structure of topological insulators ($\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.8}\text{Se}_{1.2}$ as an example) with possibility of the spin-polarized current generation along the TSS under circular dichroism (CD) photoexcitation.

One possibility of the surface spin current generation along the TSS is the use of circular polarizations of light, for instance, under the photoexcitation of electrons by the laser irradiation from low lying valence and shall core level states onto the TSS at the Fermi level. However, in our work we try to analyze other possibility of using circular polarization of light (rather synchrotron radiation with higher photon energies) for the spin current generation – due to a depopulation of the TSS at the Fermi level under photoexcitation by synchrotron radiation with opposite circular polarizations and formation of the surface spin-polarized current along the TSS compensating the holes created under photoexcitation. These holes are characterized by long relaxation time due to high bulk resistivity of TI and can stimulate some local “charging” of the place of the light spot localization and a formation of the surface spin polarized current along the TSS compensating the formed local “charging”. These processes are followed by the redistribution of electro-chemical potential between the light spot localization and the sample edges that can displays itself as an energy shift of the Fermi level in photoemission spectra measured under CD photoexcitation.

In this our work we demonstrate a possibility of experimental observation of the energy shift of the Fermi level in photoemission spectra for topological insulator $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.8}\text{Se}_{1.2}$ under photoexcitation with opposite circular polarization of synchrotron radiation and show that the shift of the Fermi level is really related to the depopulation of the TSS with opposite momentum and generation of corresponding surface spin-polarized current along the TSS in the direction perpendicular the light propagation vector. For confirmation of it we have experimentally found a correlation between the sign and the magnitude of the Fermi level shift, variation of the asymmetry of the intensity of the Dirac cone states with opposite momentum and corresponding experimentally measured current developed along the surface. The obtained results have showed that photoexcitation with different light polarizations of the system with helical spin structure can be used as for generation of the spin-polarized current along the Dirac cone states, so as for their simple registration by analysis of the experimentally observed energy shift of the Fermi level under circular dichroism photoexcitation.

Tunable Electronic Structure and Dirac Cone Warping in the Elemental Topological Insulator α -Sn

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Elemental α -Sn, in the presence of a strain-induced energy gap, was proposed to be a Topological Insulator (TI) in 2007 [1]. Recently, TI behavior was experimentally found in bulk α -Sn by our group in Würzburg [2], and also confirmed for ultrathin films [3]. This TI, like its sister compound HgTe (which was shown to exhibit the quantum spin Hall effect [4]), has a highly unusual band order: the spin-orbit coupling drives a huge band splitting, but the necessary parity inversion, which hosts the Dirac state, occurs between independent bands. The required gap in these otherwise zero-gap materials may not only be generated by strain, but also in the quantum well regime. In any case, a key question is to which extent the "topologically protected" Dirac cone may be affected in its shape and its spin texture by either the interfaces in layered structures or even by the lattice symmetry itself.

The material α -Sn can be grown on InSb(001) substrates by molecular beam epitaxy (MBE). By this means, one can also insert dopants such as Te, which allow to fine-tune the Fermi level position, e.g., to the Dirac point [2]. In our research, we have mapped out the shape of the Dirac cone, and find substantial indications that it deviates from an idealized circular shape. This is reminiscent of the bismuth telluride materials class, where an influence of the three-fold symmetry of the crystal on the spin texture and electronic properties of the topological surface state (TSS) is being discussed.

Here, we report novel data of high-quality MBE material, that allow a detailed investigation of the effect of the diamond lattice symmetry on the TSS in α -Sn. Our results from angle-resolved photoemission show that the Dirac cone is substantially modified by the (001) surface symmetry, which has an A-B stacking sequence and corresponding dimer chains. Moreover, spin-resolved photoemission reveals a lifting of the perpendicular locking of spin and momentum, while the spin remains fully within the surface plane. These surprising experimental findings are backed by extensive DFT and GW calculations of the constant energy contours.

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Characterization of the Electronic Structure along Single Bi₂Te₃ Nanowires by nano-Angle-Resolved Photoemission Spectroscopy

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The major challenge to address the surface states of topological insulator (TI) materials is the reduction of the large contribution of bulk charge carriers dominating the signals for e.g. transport measurements. Due to their high surface-to-volume ratio and controllable properties (e.g. size and composition), nanowires make excellent model systems to investigate TI surface states.

Cylindrical Bi₂Te₃ nanowires were synthesized by electrochemical deposition in the channels of ion-track etched polymer membranes. Analysis of their chemical composition and crystallographic structure by high resolution scanning electron microscopy (HRSEM), energy-dispersive x-ray spectroscopy (EDX), transmission electron microscopy (TEM), and x-ray diffraction (XRD), revealed chemically homogenous and polycrystalline, highly textured Bi₂Te₃ nanowires with grain sizes of several hundreds of nm [1].

Single nanowires were investigated by nano-angle-resolved photoemission spectroscopy (nanoARPES) at the ANTARES beamline at the SOLEIL Synchrotron, which provides a resolution in the sub-micron range. In particular, cylindrical Bi₂Te₃ wires of 100 nm diameter and length of up to 30 µm were fabricated. They were randomly distributed on a p-doped silicon substrate by wet chemical dissolution of the surrounding polymer membrane and subsequent drop casting. The cleanness of the sample's surface after the transfer process was evaluated by core level spectroscopy and nanoARPES to identify oxygen and carbon contamination and the quality of the band structure, respectively.

By combining scanning and on-focus operation ARPES modes, individual nanowires were imaged using both Te 4d core level and top of the valence band signals. ARPES measurements were conducted on several points along several selected single wires. The band structures indicate that the Fermi level of these nanowires lies within the valence band. Interestingly, different valence band structures were obtained depending on the position on a given wire. The interpretation and the origin of these differences are still under investigation.

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Non-Dirac topological surface states in $(\text{SnTe})_{n>1}(\text{Bi}_2\text{Te}_3)_{m=1}$

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A new type of topological spin-helical surface states was discovered in layered van der Waals bonded $(\text{SnTe})_{n>1}(\text{Bi}_2\text{Te}_3)_{m=1}$ compounds which comprise two covalently bonded band inverted subsystems, Bi_2Te_3 and SnTe — well known time-reversal and crystalline topological insulators (TIs). In $(\text{SnTe})_n(\text{Bi}_2\text{Te}_3)_m$ series [1] the $(n = 1, m > 1)$ compounds — SnBi_4Te_7 , $\text{SnBi}_6\text{Te}_{10}$, and $\text{SnBi}_8\text{Te}_{13}$ are structurally identical to earlier studied lead-based TIs [2], containing alternating QL and SL structural units, while the $(n > 1, m = 1)$ compounds are formed by unique, nonalternating building blocks. The superposition of two pairs of SOI-induced band inversions realized in SnTe and Bi_2Te_3 subsystems gives rise to the formation of two spin-helical topological surface states at the Γ point. These states reside in the band gap and in the local gap of the valence band.

The bandgap topological state demonstrates novel non-Dirac dispersion with two linear sections of different slope and very low-velocity shoulder section between them. Thus in contrast to all hitherto known topological insulators, where the slope of the spin-helical surface state is linear or varies smoothly with energy, the bandgap topological surface state in $(\text{SnTe})_{n=2,3}(\text{Bi}_2\text{Te}_3)_{m=1}$ compounds shows abrupt switch of the velocity of topological carriers with change in the Fermi surface topology in the narrow energy range (shoulder section) where spin and charge current should be blocked. This novel finding enhance the understanding on the diversity of topological surface states and pave a way for the efficient control of the group velocity with sufficiently large spin current density by tuning the chemical potential. Further tuning of the bandgap surface state parameters can be realized by using $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ or $\text{Bi}_2(\text{Te}_{1-x}\text{Se}_x)_3$ compounds as basic TIs for construction of $(\text{SnTe})_{n>1}((\text{Bi-Sb})_2(\text{Te-Se})_3)_{m=1}$ systems.

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Dirac States On The Noncentrosymmetric BiPd Surface

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Materials with strong spin-orbit coupling (SOC) have in recent years become a subject of intense research efforts due to their potential use for spin-based devices and quantum information technology [1]. In noncentrosymmetric materials, strong SOC modifies the bulk and surface band structures in various ways [2,3]. First, due to the Rashba effect it lifts the spin degeneracy of bulk and surface bands, generating intricate spin textures in the electron Bloch wave functions. Second, strong SOC can shift the conduction and valence bands in opposite directions, giving rise to an inverted band structure with non-trivial topological Dirac surface states [4–7].

Here, by combining relativistic first-principles band calculations with ARPES measurements we examine the role of spin-orbit coupling in noncentrosymmetric BiPd single-crystals [8–10]. We report the detection of several Dirac surface states at different binding energies and with very large Rashba-splitting. Unlike the surface states in inversion-symmetric systems, the Dirac surface states of BiPd have quite different properties at opposite sides of the crystal. Our ARPES measurements agree well with the calculated band structure of the inequivalent (010) and (0-10) surfaces of BiPd.

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Giant Rashba Splitting in (111) $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ Topological Crystalline Insulator Epilayers Induced and Tuned by Bi Doping

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3D topological crystalline insulators (TCIs) with 2D topological surface states (TSSs) protected by $\{110\}$ mirror plane symmetry have been recently discovered in the lead-tin chalcogenide material family. In comparison to Z_2 topological insulators, TCIs feature enhanced tunability of TSSs by external perturbations such as temperature, composition, strain as well as electric and magnetic fields, which provides a basis for observation of novel effects and future applications [1]. In majority of previous works, bulk TCI crystals cleaved along the $\{001\}$ natural cleavage planes of the lead tin chalcogenides were studied, while TSSs of other planes such as $\{110\}$ or $\{111\}$ have remained relatively unexplored. Due to polar nature of $\{111\}$ plane one would expect different properties of the TSS in comparison to the non-polar $\{001\}$ plane which contains equally both cations and anions [2].

In this work, we have studied the $\{111\}$ TSSs of $(\text{Pb}_{1-x}\text{Sn}_x)_{1-y}\text{Bi}_y\text{Te}$ epilayers grown by molecular beam epitaxy using ARPES at the at UE112_PGM-2a-1^{^2} beamline of BESSY II. The high intrinsic p-type carrier concentration due to Pb/Sn vacancies in $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ was compensated by Bi doping that allowed us to obtain n-type samples and thus, to observe the conduction and valence bands. We find a gap closing for x_{Sn} larger than about 45 % at low temperatures. Moreover, a giant Rashba splitting is observed for the valence band while conduction band remained unsplit (see Fig. 1). In particular, we find that Rashba splitting increases with increasing Bi concentration and it is absent for undoped epilayers. The values of k_0 -splitting and Rashba parameter for the sample doped with 0.66 % Bi are as large as $k_0=0.017\text{\AA}^{-1}$ and $\alpha_R=3.5\text{ eV\AA}$, comparable to the values reported for other giant Rashba splitted systems [3].

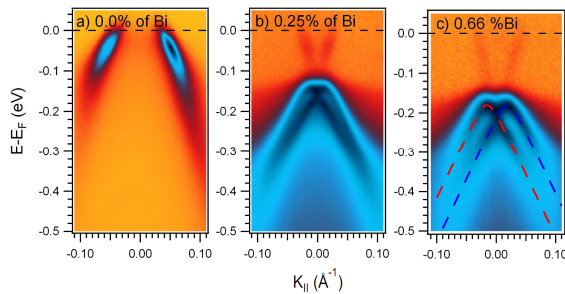


Fig. 1: ARPES $E(k)$ spectra of (111) $\text{Sn}_{0.46}\text{Pb}_{0.54}\text{Te}$ epilayers with different Bi doping concentrations, ranging from 0 to 0.66 % from left to right, measured at 100K with photon energy of 18 eV. The lines in (c) are guide to eyes.

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Two-dimensional weak antilocalization in topological crystalline insulator SnTe thin films

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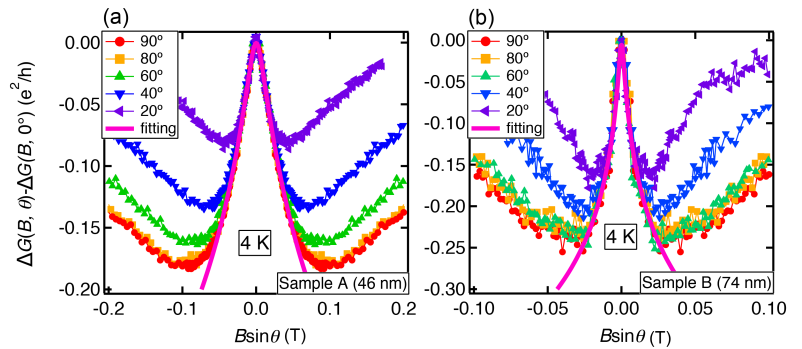
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SnTe has been attracting attention as a topological crystalline insulator (TCI), in which the surface state is protected by the mirror symmetry of the crystal, instead of the time-reversal symmetry in a conventional topological insulator[1]. Some of the transport properties of the surface state have also been reported in SnTe[2-4], but the intrinsic topological surface state on a trivial insulator has not been confirmed so far.

In this study, we have investigated the surface transport in detail. We grew SnTe thin films on a BaF₂(111) substrate by optimizing the growth conditions.

The analysis of the Hall conductivity measured on the grown films reveals that two types of carriers, one in bulk and the other in the surface state, contribute to the electric transport. By decreasing the thickness of the SnTe layer down to 46 nm, we achieved low carrier densities of $1.1 \times 10^{18} \text{ cm}^{-3}$ in bulk and $6.0 \times 10^{11} \text{ cm}^{-2}$ in the surface state at 4K. In the magnetoresistance (MR) measurement, we observed a positive sharp peak in the MR curve at low temperatures below 15K originating from the weak antilocalization (WAL) effect [5]. Since the WAL effect arises not only in the two-dimensional (2D) transport on the topological surface but also in the bulk transport in the existence of strong spin-orbit interaction, we extract the 2D component arising from the surface transport by analyzing the dependence of MR on the angle of an applied magnetic field, as the result at 4K is shown in Fig.1. In this figure, the MR under an in-plane magnetic field is subtracted from the MR under a magnetic field B of the respective angles θ against the film plane and plotted as a function of $B \sin \theta$. The subtracted MR falls on one universal curve, which is attributed to the 2D component of the WAL in the surface transport. From the fitting of this curve to the theoretical equation, we obtain the parameter α related to the number of transport channels and the phase coherence length l_ϕ . The analysis of the MR measured at different temperatures reveals that l_ϕ exhibit different temperature dependences between the thin (46nm) and thick (74nm) films, suggesting different scattering mechanisms between the two films; the electron-electron scattering in the thin film and the electron-phonon scattering in the thick film. The dominance of the electron-electron scattering in the thin film is considered to be peculiar to the 2D transport on the surface state, similarly to that reported in bismuth thin films[6].



The extracted 2D WAL in thin (a) and thick (b) films.

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HgTe as a Topological Insulator

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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[4,5]. Due to the screening properties of Dirac fermions, these states turn out to be decoupled from the bulk for a very wide range of densities[5]. This allows us to induce a supercurrent in the surface states by contacting these structures with Nb electrodes[6]. AC investigations indicate that the induced superconductivity is strongly influenced by the helical character of the charge carriers.

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“Spotting the elusive Majorana under the microscope”

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Topological superconductors are a distinct form of matter that is predicted to host boundary Majorana fermions. The search for Majorana quasi-particles in condensed matter systems is motivated in part by their potential use as topological qubits to perform fault-tolerant computation aided by their non-Abelian characteristics. Recently, we have proposed a new platform for the realization of Majorana fermions in condensed matter, based on chains of magnetic atoms on the surface of a superconductor. This platform lends itself to measurements with the scanning tunneling microscope (STM) that can be used to directly visualize the Majorana edge modes with both high energy and spatial resolution. Using rather unique STM instrumentation, we have succeeded in creating this platform and have observed the predicted signatures of localized Majorana edge modes. I will describe our Majorana platform, the experiments to date, and the outlook for further experiments on Majorana fermions in our platform.

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Strong localization of Majorana end states in chains of magnetic adatoms

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A recent experiment [1] gives possible evidence for Majorana bound states in chains of magnetic adatoms placed on a superconductor. While many features of the observed end states are naturally interpreted in terms of Majoranas, their strong localization remained puzzling. Based on general heuristic arguments as well as a detailed model calculation, we show that Majorana states in proximity-coupled systems may be localized on a scales much smaller than the coherence length of the host superconductor as a consequence of a strong velocity renormalization [2].

Specifically, we consider a linear chain of Anderson impurities on a superconductor as a minimal model and treat it largely analytically within mean-field theory. We explore the phase diagram, the subgap excitation spectrum, and the Majorana wavefunctions.

Evidence for Majorana bound states in experiments such as in Ref. [1] largely relies on measurements of the tunneling conductance. While the conductance into a Majorana state is in principle quantized to $2e^2/h$, this quantization is difficult to observe due to thermal broadening in the normal-metal lead. We propose to use a superconducting lead instead, whose gap strongly suppresses the effects of temperature broadening. A Majorana state leads to symmetric conductance peaks at $eV = \pm \Delta$ which have the universal height $G = (4-\pi) 2e^2/h$ for a wide range of tunneling strengths and temperatures [3]. For a superconducting scanning tunneling microscope tip, Majorana states therefore appear as a spatial conductance plateau, while the conductance varies with the local wavefunction for a trivial fermionic bound state. We also discuss effects of nonresonant (bulk) Andreev reflections and quasiparticle poisoning.

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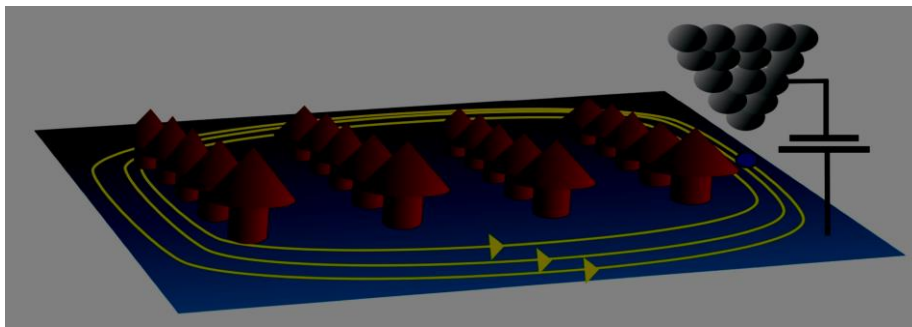
Exotic topological superconductivity and high Chern numbers in lattices of magnetic adatoms on a superconductor

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Magnetic adatoms deposited on a surface of an ordinary s-wave superconductor has been predicted to support topological superconductivity. Recent STM experiments indeed exhibit signatures of Majorana end states in ferromagnetic chains [1]. This has launched an avalanche of interest towards these systems. In principle these systems could serve as a highly tunable platform to study topological superconductivity and Majorana physics.

Going beyond the much studied case of 1D chains, we anticipate further developments in the field by studying 2D lattices of magnetic atoms. We consider so-called dilute Shiba limit where the orbitals of the magnetic atoms do not have a direct overlap. Assuming a ferromagnetic ordering combined with a strong Rashba spin-orbit coupling on the surface, we predicted that these systems support chiral topological superconductivity generalizing the much sought-after $p+ip$ pairing state [2]. Remarkably, we have found that for typical physical parameters these systems can realize superconducting states with very high Chern numbers $C \gg 1$. Due to the bulk-boundary correspondence, these systems also support a large number of dispersive Majorana edge states.

I will discuss how 2D magnetic lattices on a superconducting surface realize very complex topological phase diagrams and how the consequences could be observed in STM experiments. I will also explain how fabrication of 2D lattices of magnetic atoms on superconducting surfaces will open up a possibility to create designer 2D topological superconductors with high Chern numbers and large number of edge modes.



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Search for additional signatures of Majorana fermions in semiconductor nanowires coupled to superconductors

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I will provide and update on the experiments in InSb nanowires coupled to superconductors. The talk will focus on tunneling experiments and the analysis of zero-bias peaks, induced gaps and methods of the preparation of clean transparent contacts between superconductors and semiconductors. Near term goals include the search for the closing of the topological superconducting gap, correlations between zero-bias features, phase diagrams of the topological states.

Non-contact current-phase measurements of topological weak links with scanning SQUID

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We use Superconducting QUantum Interference Device (SQUID) microscopy to characterize the current-phase relation (CPR) of Josephson Junctions from the 3-dimensional topological insulator HgTe (3D-HgTe). We find clear skewness in the CPRs of HgTe junctions ranging in length from 200 nm to 600 nm. The skewness indicates that the Josephson current is predominantly carried by Andreev bound states with high transmittance, and the fact that the skewness persists in junctions that are longer than the mean free path suggests that the effect may be related to the helical nature of the Andreev bound states in the surface of HgTe. These experimental results suggest that the topological properties of the normal state can be inherited by the induced superconducting state, and that 3D-HgTe is a promising material for realizing the many exciting proposals that require a topological superconductor. These measurements showcase the CPR as a fundamental characteristic of superconducting weak links and establish scanning SQUID microscopy as a powerful probe for performing such measurements.

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Unconventional Current-Phase Relation in Coplanar Proximity Devices

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Proximity induced superconductivity in devices where the barrier consists of a Topological Insulator (TI) has recently become of great interest for the possibility to study a variety of new phenomena including Majorana Fermions physics [1, 2]. At the early stages of the field, most of the efforts to detect Majorana fermions were centered in finding evidences of a 4π periodic current phase relation (CPR) [1, 3]. Later on, further studies revealed that the theoretical scenario is much more complex than expected [4]. In fact, parity-switching processes, mainly determined by quasiparticle poisoning, are expected to mask most of the effects related to the 4π periodicity [3, 4, 5]. However, when the switching processes are extremely abundant, some unconventional features can be addressed, as for instance in the noise properties of the devices at very high frequencies [4], or in the magnetic response of the device [5]. In this respect, a $0-\pi$ transition [5] is expected to manifest in S/TI/S proximity devices, at high levels of the quasiparticle poisoning.

Here we report on the transport characterization of coplanar proximity devices with Al superconducting electrodes and the 3D topological insulator Bi_2Te_3 as a barrier. The measurements presented here refer to Josephson junctions and dc SQUIDs. In particular we have studied the current voltage characteristics as a function of an external magnetic field, and of a microwave field. In such devices we have detected the possible occurrence of an unconventional CPR with higher order harmonics, manifesting as a dip in the magnetic pattern at zero external field, together with the appearance of non-integer Shapiro steps.

In particular the overall shape of some of the magnetic pattern resembles that of a $0-\pi$ Josephson junction [6]. Recently, evidences of higher harmonics on HgTe heterostructures have also been claimed [7], consistently with our measurements.

The correlation between the transport properties and the film morphology is also discussed, addressing some features that enhanced the proximity in the film and therefore the Josephson coupling. These features might be connected to the intrinsic and extrinsic strain of the topological insulator, as pointed up in recent papers [8, 9].

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The electronic structure of superconducting Cu intercalated Bi₂Se₃

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Recently, superconductivity was found in Cu intercalated Bi₂Se₃ with a T_c of about 4K [1]. This caused excitement in the community, as it is believed that this system is the first example of a topological superconductor, a superconductor that has non-trivial topological properties.

Fu and Berg [2] have provided a sufficient criterion that can be used to identify time reversal invariant 3D topological superconductors. A superconductor that has an odd-parity order parameter and that its Fermi-surface encloses an odd number of Time Reversal Invariant Momenta (TRIM) points is a 3D topological superconductor.

Evidence for non-trivial superconductivity in Cu_xBi₂Se₃ was provided by point-contact spectroscopy. The spectra have shown Zero Bias Conductance Peaks (ZBCP) [3,4], which is believed to be a signature of dispersive Majorana modes [5].

On the other hand, we have recently shown that Cu_xBi₂Se₃ [6] does not satisfy the Fu and Berg criterion since its Fermi-surface encloses two TRIM points. This leaves a few open questions: What is the origin of the ZBCPs? Can it be that Cu_xBi₂Se₃ is a different kind of a TSC? Can Cu_xBi₂Se₃ be a 2D TSC?

We try to answer these questions by performing ARPES experiments using better crystals. Using an electro-chemical intercalation method [3] to prepare Cu_xBi₂Se₃ we managed to increase the superconducting volume fraction of our crystals to about 90%. The ARPES spectra of these crystals are very different than the spectra of Bi₂Se₃ and from the spectra of previously studied Cu_xBi₂Se₃.

We find this kind of spectra only in 1 out of 10 measurements. We suggest that this new spectra represents the superconducting samples and explain why superconductivity in Cu_xBi₂Se₃ is so elusive.

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Lateral heterojunctions on inverted HgTe quantum wells

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We study lateral heterojunctions on HgTe quantum wells with inverted band structure. At zero magnetic field we observe a set of oscillations that resemble the Fabry-Perot interference patterns observed for other 2DEG systems, such as graphene [1]. In the bulk gap, the interference pattern could be due to bouncing of Quantum Spin Hall states at the junction.

At high densities and applied magnetic field, we can explore the equilibration between Quantum Hall (QH) states with different filling factor. The resulting resistance plateaus are particularly clear in the n - n' - n quadrant and fit the expected values for a 2D electron gas heterojunction [2,3].

The low density and moderate magnetic field regime is of more interest, since due to the inverted band structure of HgTe, Quantum Spin Hall (QSH) edge states could be present under broken time reversal symmetry [4]. In this regime, we can explore the equilibration between QSH and QHE edge states, as preliminary done by Gusev et al. [5]. In addition we observe unexpected features in the Hall resistance, which could be associated with the interplay between chiral QH edge modes and helical QSH edge modes.

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Crossed surface flat bands of Weyl semimetal superconductors

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Topological superconductor with time reversal symmetry is a hot topic now. Recently, topological superconducting state has been predicted in Cu doped Bi₂Se₃ (Cu_xBi₂Se₃)[1]. Point contact spectroscopy has shown a zero bias conductance peak (ZBCP) consistent with the presence of surface edge mode[2], i.e., surface Andreev bound states (SABSs)[2]. We have developed a theory of the tunneling spectroscopy for superconducting topological insulators (STIs), where the SABSs appear as helical Majorana fermions. We have found that the SABSs in the odd-parity STIs have a structural transition in the energy dispersions. The transition [3,4] results in a variety of Majorana fermions, by tuning the chemical potential and the effective mass of the energy band. We further derived an analytical formula of the conductance of the present junction [6] which is an extension of the conductance formula of unconventional superconductors [7]. The origin of this anomalous dispersion stemming from the residual surface density of states in topological insulator.

Residual density of states plays an important role in Weyl semimetal where Fermi arc exists in the normal state[8-9]. In this presentation, we will explain new type of surface Andreev bound state in doped Weyl semimetal superconductor. It has been noted that certain surfaces of Weyl semimetals have bound states forming open Fermi arcs, which are never seen in typical metallic states. We show that the Fermi arcs enable them to support an even more exotic surface state with crossed flat bands in the superconducting state. We clarify the topological origin of the crossed flat bands and the relevant symmetry that stabilizes the cross point[10]. Our symmetry analysis are applicable to known candidate materials of time-reversal breaking Weyl semimetals. We also discuss their possible experimental verification by tunneling spectroscopy.

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Topologically protected charge transfer along the edge of a chiral p-wave superconductor

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Since Majorana fermions are charge neutral, quantized electrical signatures of them are lacking. We calculate the full counting statistics of the transferred charge of Majorana fermions propagating along the edge of a topological superconductor with $p+ip$ pairing and find that it becomes trinomial in the low-temperature limit, distinct from the binomial statistics of charge- e transfer in a single-mode nanowire or charge- $2e$ transfer through a normal-superconductor interface. All even-order correlators of current fluctuations have a universal quantized value, insensitive to disorder and decoherence. We propose these as macroscopic signatures of the Majorana edge mode, persisting on energy scales large compared to the Thouless energy.

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Pseudo-ballistic Transport in 3D Topological Insulator Quantum Wires

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Disorder strongly alters the nature of charge transport in nanostructures, with a crossover from ballistic to diffusive transport when impurities are introduced into a mesoscopic conductor¹. Unlike massive quasi-particles, Dirac fermions can induce exotic situations for which ballistic and diffusive properties are not distinctive. Thus, signatures of diffusion were found in ballistic graphene nanostructures at the Dirac point, corresponding to pseudo-diffusive transport.

Here, we reveal ***a new transport regime for which ballistic properties persist well beyond the transport mean free path***, characteristic of diffusive transport. This pseudo-ballistic regime is evidenced by non-universal conductance fluctuations of highly-doped and strongly-disordered Bi₂Se₃ nanowires at very low temperatures: using a 3D-vector superconducting magnet, we measured the quantum corrections to the classical conductance along a perpendicular direction with respect to the axis of the nanowire for different values of the parallel magnetic field. Contrary to the expected diffusive case, the amplitude of the conduction fluctuations is found to be strongly modulated by the parallel magnetic field.²

Theory is able to reproduce the modulation of the conductance fluctuations and reveals that spin helical Dirac fermions in quantum wires retain pseudo-ballistic properties over an unusually broad energy range, due to strong quantum confinement and weak scattering.²

These findings highlight the remarkable and subtle interplay of topological quasi-particles in 3D topological insulators with disorder in a mesoscopic conductor.

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Two-Dimensional Topological Insulator Edge State Backscattering by Dephasing

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Edge transport in 2d topological insulators is protected from elastic backscattering by time-reversal symmetry, which promises exceptionally robust low-temperature transport properties. However, state-of-the-art experiments observe significant edge-state backscattering, the mechanism of which is still unknown. In particular, all these experiments have in common that the backscattering strength is almost temperature independent, which seems to rule out most inelastic backscattering mechanisms.

We theoretically investigate one mechanism that might explain the observed temperature-independent backscattering: a combination of an inelastic interaction which is responsible for breaking the electron phase coherence (dephasing) in combination with elastic backscattering in quantum dots (puddles, which are naturally expected in these materials because of potential fluctuations due to trapped charges). Using analytical models and new numerical techniques, which allow to calculate electron dynamics in the presence of dephasing, we quantitatively estimate the importance of this mechanism in HgTe/CdTe quantum wells. We find that it is compatible with and could provide the key to the observed temperature-independent resistance if the quantum dots in the sample are large or weakly coupled to the edge.

Vice versa, using small (≈ 100 nm) artificial quantum dots which can be controlled in depth, one should be able to observe a detectable temperature dependence from which the actual dephasing time scale in the material could be inferred using our data. This could, e. g., be achieved by structuring the quantum wells using gates.

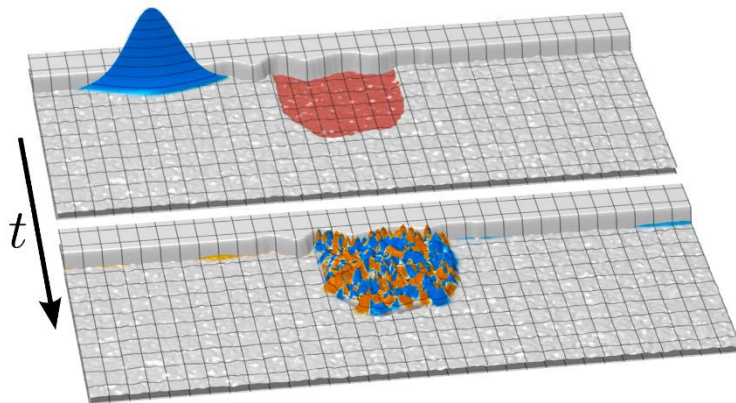


Figure 1: Snapshots of our calculations in which a wave packet (the color encodes the spin) approaches a puddle at the edge of a 2d TI. In the puddle, the wave function becomes fully spin-mixed (due to spin-orbit coupling) such that even a spin-conserving dephasing event leads to backscattering.

Low carrier concentration crystals of the topological insulator $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$: a magnetotransport study

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In 3D topological insulators the bulk conduction channel shunts and masks the topological transport properties. To achieve a genuine bulk-insulating state is an important research topic. Recently, the material system $(\text{Bi,Sb})_2(\text{Te,Se})_3$ (BSTS) has been proposed as a topological insulator with high resistivity and a low carrier concentration [1]. Here we present a study to further refine the bulk-insulating properties of BSTS [2]. We have synthesized two series of $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$ single crystals: (i) x varies from 0.42 to 0.58 and y is fixed at 1.3, and (ii) x is fixed at 0.54 and y varies from 1.2 to 1.6. Resistance and Hall effect measurements show that a record high bulk-insulating behavior with resistivity of $12.6 \, \Omega \, \text{cm}$ combined with a low carrier density around $2 \times 10^{15} \, \text{cm}^{-3}$ can be achieved for the composition $\text{Bi}_{1.46}\text{Sb}_{0.54}\text{Te}_{1.7}\text{Se}_{1.3}$ at 4.2 K. In order to disentangle the surface and bulk contributions we have measured the resistance for crystals $\text{Bi}_{1.46}\text{Sb}_{0.54}\text{Te}_{1.4}\text{Se}_{1.6}$ with thicknesses between 6 and 140 micrometer. The analysis of the resistivity within a parallel resistor model shows that the bulk and surface conductivities are $0.053 \, \Omega^{-1} \, \text{cm}^{-1}$ and $318 \, \Omega^{-1} \, \text{cm}^{-1}$ respectively. Therefore, when the sample thickness is reduced to 1 micrometer the surface contribution to the electrical transport amounts to 97 % and surface dominated transport can be achieved. The magnetoconductance of an exfoliated $\text{Bi}_{1.46}\text{Sb}_{0.54}\text{Te}_{1.7}\text{Se}_{1.3}$ nanoflake with a thickness of 130 nm has been measured in the temperature range from 2 to 40 K. Based on the analysis with the Hikami-Larkin-Nagaoka model, the magnetoconductance shows 2D weak antilocalization with the fit parameter α close to -1 as expected for transport dominated by topological surface states. Furthermore, Shubnikov - de Haas oscillations on crystals with composition $\text{Bi}_{1.46}\text{Sb}_{0.54}\text{Te}_{1.7}\text{Se}_{1.3}$ and $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$ have been observed in magnetic fields up to 30 T and show 2D electronic states. The Landau level fan diagram shows a finite Berry phase, the hall mark for topological surface states. By using the Lifshitz-Kosevich formalism, important transport parameters of the surface states, such as the carrier density, cyclotron mass and quantum mobility, were obtained.

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Ferromagnetic topological insulator and quantum transport

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In topological insulators (TI) the Dirac surface states are induced by the strong spin-orbit coupling (SOC) as well as protected by the time reversal symmetry (TRS). Breaking TRS in a TI with ferromagnetic perturbation can lead to many exotic quantum phenomena including the quantum anomalous Hall (QAH) effect. The spontaneously broken TRS states can be introduced into TI by ferromagnetic ordering, achievable by two methods: i) conventional way, by doping with a magnetic element, ii) by ferromagnetic proximity coupling. We shall describe our experimental studies in both approaches showing unexpected interfacial behavior as well as van Vleck ferromagnetism. The exotic QAH state describes the dissipationless quantized Hall transport in ferromagnetic materials in the absence of external magnetic fields. The realization of the QAH effect in realistic materials required two conditions: ferromagnetic insulating materials and topologically non-trivial electronic band structures. We shall describe how in a hard ferromagnetic TI system a robust QAH state and dissipationless edge current flow is achieved.¹ The realization of QAH state and the occurrence of dissipationless conduction in hard ferromagnetic TIs could be a major step towards dissipationless electronic applications in the absence of external fields, making such devices more amenable for metrology and spintronics applications.

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Topological Insulators with Magnetic Texture

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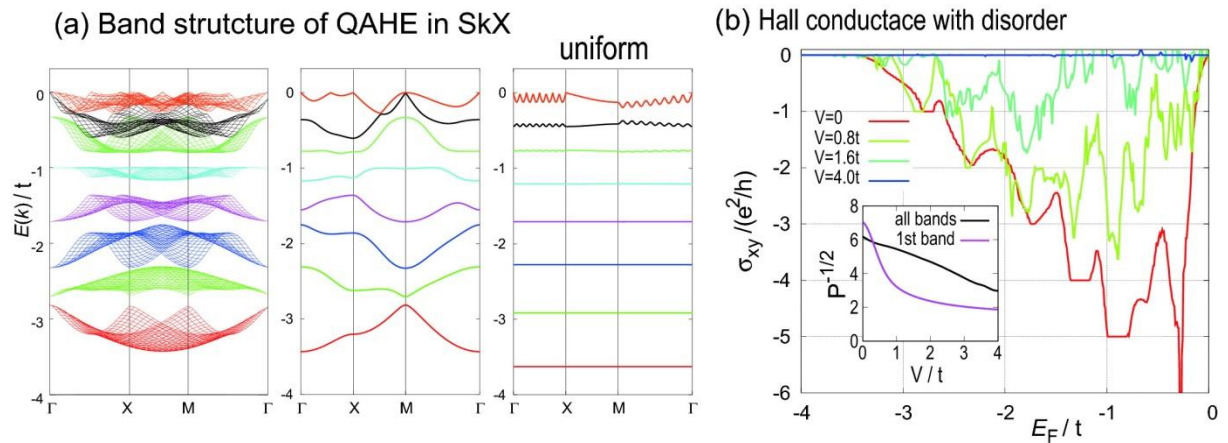
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Topological insulators (TIs) show rich phenomena and functions which can never be realized in ordinary insulators. Most of them come from the peculiar surface or edge states. Especially, the quantized anomalous Hall effect (QAHE) without an external magnetic field is realized in the two-dimensional ferromagnet on a three-dimensional TI which supports the dissipationless edge current[1,2]. Here we demonstrate theoretically that the domain wall of this ferromagnet, which carries edge current, is charged and can be controlled by the external electric field. The chirality and relative stability of the Neel wall and Bloch wall depend on the position of the Fermi energy as well as the form of the coupling between the magnetic moments and orbital of the host TI. These findings will pave a path to utilize the magnets on TI for the spintronics applications. We also discuss the quantum anomalous Hall effects with magnetic textures.

We also study the QAHE in skyrmion crystal (SkX) without external magnetic field. The emergent magnetic field in SkX could be gigantic as much as 4000T when its lattice constant is 1nm. The band structure is not flat but has a finite gap in the low electron-density regime. We also study the conditions to realize the QAHE for the skyrmion size, carrier density, disorder strength and temperature. Comparing the SkX and the system under the corresponding uniform magnetic field, the former is more fragile against the temperature compared with the latter since the gap is reduced by a factor of 1/5, while they are almost equally robust against the disorder. Therefore, it is expected that the QAHE of SkX system is realized even with strong disorder at room temperature when the electron density of the order of one per a skyrmion.



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Surface Dirac fermion dynamics of non-magnetic and magnetic topological insulators

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Topological insulators (TIs) are a new quantum state of matter. Their surfaces and interfaces act as a topological boundary to generate massless Dirac fermions with spin-helical textures. Furthermore, magnetically doped topological insulators, possessing an energy gap created at the Dirac point through time-reversal-symmetry breaking, are predicted to exhibit exotic phenomena including the quantized anomalous Hall (QAH) effect. Although several candidates of magnetically doped TIs were demonstrated to show long-range magnetic order, the realization of the QAH effect is so far restricted to V- and Cr-doped $(\text{Sb,Bi})_2\text{Te}_3$ systems at extremely low temperature [1, 2]; however, the microscopic origin of its ferromagnetism is poorly understood. Besides, investigation of fermion dynamics near the Dirac point is crucial for the future development of spintronic devices incorporating topological insulators.

Angle-resolved photoemission spectroscopy implemented by a pump-and-probe method (TrARPES) is a powerful tool to study the unoccupied states and electron dynamics with energy, momentum and time resolutions. First, we have explored the surface Dirac fermion dynamics in the topological insulator Sb_2Te_3 and the related p -type TIs. Sb_2Te_3 has a Dirac node completely located above the Fermi energy. The excited electrons in the upper Dirac cone stay longer than those below the Dirac node to form an inverted population. This is attributed to a reduced density of states near the Dirac node [3]. Second, we present an element-resolved study for V and Cr-doped $(\text{Sb,Bi})_2\text{Te}_3$ using X-ray magnetic circular dichroism to unambiguously show that the long-range magnetic order is mediated by the p -hole carriers of the host lattice, and the interaction between the Sb (Te) p and V(Cr) d states is crucial [4]. Our results are important for material engineering in realizing the QAH effect at higher temperatures. TrARPES experiment has also been applied to these magnetic topological insulators. The surface Dirac cones are clearly observed for all the studied samples. We will also discuss time evolution of the pumped Dirac electrons of these magnetic TIs.

The XMCD experiment was performed at SPring-8 under the Shared Use Program of JAEA Facilities (Proposal No. 2013A-E10, 2013B-E32) with the approval of Nanotechnology Platform project supported by the Ministry of Education, Culture, Sports, Science and Technology (Proposal No. 2013A3880 and 2013B3880). The TrARPES measurements were jointly carried out at the LASOR of the Institute for Solid State Physics, the University of Tokyo (Proposal No. A181, A184).

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Quantized Hall effects in topological insulator field-effect transistor

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Topological insulator is a novel state of matter characterized by two-dimensional metallic Dirac states on its surface. Quantization of the Dirac surface states is of great interest to verify the topological nature in three dimensional topological insulator (3D-TI). In our study, we performed electrical measurement on the field-effect transistor based on $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ thin films. Integer quantum Hall effect is observed at $\nu = \pm 1$ under applying magnetic field. By tuning the composition x along growth direction in the films, $\nu = 0$ quantized state in Hall conductivity is revealed owing to the difference of the energy levels of top and bottom Dirac points. In addition, when Fermi energy of ferromagnetic Cr doped $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ is well-controlled via field-effect gating, quantization of anomalous Hall effect is achieved in electrical characterization under zero magnetic-field, verifying the exchange gap in Dirac surface state. In the talk, I will discuss on the quantized transport properties of the field-effect transistor based on non-magnetic TI [2], magnetic TI [1] and bilayer stacked with these two TIs [3].

This study has been carried out in RIKEN CEMS and Univ. Tokyo under the collaboration with R. Yoshimi, K. Yasuda, M. Mogi, Y. Kozuka, J. Falson, J. G. Checkelsky, K. S. Takahashi, N. Nagaosa, M. Kawasaki, and Y. Tokura.

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Magnetism and topological insulators

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It is a well known fact that a magnetic field can break the time reversal symmetry and therewith can destroy a topologically protected surface state in topological insulators. However, the interplay between magnetism and topological order can yield a number of interesting phenomena such as the quantum anomalous Hall effect, a topological magnetoelectric effect, and quantized Kerr- or Faraday rotation. This motivates researcher for a search of new magnetic topological insulators and for an intensive study of their electronic and magnetic properties. In my talk, I'll give an overview of our first-principles investigations on this class of materials. In the first part, I'll present a method and approximations used in our simulations and then talk about several examples of magnetic topological insulators, studied in our group within the last three years. First of all, I'll discuss topological insulators doped with magnetic impurities, which can imply various magnetic order in these materials. A special attention will be devoted to the exchange interaction between magnetic impurities and to the impact of electron-magnon interaction on the electronic structure in some doped topological systems. As next, I'll demonstrate how some defects or impurities without magnetic moments can induce magnetism in topological insulators and discuss the main features of magnetic interactions in these systems.

MAGNETIC IMPURITIES AND MAGNETOTRANSPORT IN ULTRATHIN CRYSTALLINE BI FILMS

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The surface of Bi as a semi-metal with strong spin-orbit coupling has many similarities to topological insulators (TI). Using ultrathin films, conductance is reduced to pure surface conductance also for the non-TI material Bi at low temperatures, since the bulk states become gapped due to robust confinement. It is therefore attractive to study the magnetoconductive properties of the Bi(111) surface, also in presence of magnetic impurities of Cr, Co, Fe and Tb, in the range of a few percent of a monolayer. These results will finally be compared with similar measurements for the TI material $\text{Bi}_{1-x}\text{Sb}_x$ with x around 0.18.

A central topic is the scattering of electrons within these spin-polarized surface states because time-reversal symmetry (TRS) requires a suppression of direct backscattering of charge carriers between states with opposite wave vectors and spin orientations. On the other hand, scatterers with strong spin-orbit coupling allow to change both spin and momentum so that this rule may be violated. Therefore, we measured surface state magnetoconductance and Hall effect on epitaxial Bi(111)-films, in combination with low-energy electron diffraction, and in presence of small concentrations (up to 10% of a monolayer, ML) of Bi, Fe, Co, Cr and Tb atoms, which exhibit various binding strengths and residual magnetic moments. All 3d transition metal atoms are bound at lower edge of the first Bi double layer, a position they reach without activation barrier, whereas Bi and Tb stay on the surface. Magnetoconductance is characterized by considerable charge transfer (0.03 e/atom for Cr up to 0.5 e/atoms for Fe and Co), reduction of mobilities and strong spin-orbit scattering, thus explaining sign reversals of the Hall resistance, as well as a reduction of the weak anti-localization (WAL) effect in all cases. WAL is even reversed into weak localization for Fe, Co and Cr, demonstrating strong intermixing of spin and (orbital) momentum. The scattering power of the atoms scales roughly with the binding energy, whereas scaling of the WAL to WL transition depends on the residual magnetic moment. Interestingly, the high magnetic moment from the f-electrons of Tb ($10 \mu_B$) turned out to be almost irrelevant so that Tb was the weakest scatterer of all atoms investigated. Surface diffusion, however, is non-negligible even at temperatures of 10 K for Tb and Cr. Tb adatoms finally nucleate at intrinsic defects of the Bi(111) surface, where the Tb impurities act as dopants, but not as scatterers.

Qualitatively very similar effects have been found for the TI $\text{Bi}_{1-x}\text{Sb}_x$ with $x=0.18$ at temperatures below 30 K and for a layer thickness above 8 nm. Due to alloying, surface mobilities are reduced. Contrary to pure Bi, Cr now acts as a strong acceptor, demonstrating the subtleties of electronic interactions.

Interactions of Topological (Crystalline) Insulators with Superconductivity and Magnetism

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Topological insulators (TI) are a new class of insulators with the inverted bulk gap due to strong spin-orbit coupling. On their interfaces with ordinary insulators, gapless states inevitably occur. 3D TIs have surface states (SS) with an odd number of massless Dirac cones with the spin-momentum locked electrons. In related topological crystalline insulators, the existence and protection of SS is dictated by symmetries of the underlying lattice. The physics of TIs is even more interesting with the inclusion of correlations: when interacting with magnetism or superconductivity, TIs and TCIs are predicted to show a variety of highly unusual phenomena, ranging from induced magnetic monopoles, quantum anomalous Hall effect, $p+ip$ superconducting order parameter, Majorana and Weyl fermions, etc. Some of these exotic phenomena might be used for spintronics applications, magnetic recording and quantum computing, but problems with materials and very stringent constraints on physical parameters render the wide-spread applications extremely difficult. Therefore, both the materials synthesis and the physical parameters constraints have to be explored and optimized. Here, we present the angle and spin resolved photoemission spectroscopy studies of various *in-situ* grown TI and TCI hetero-structures involving interfaces with magnetic and superconducting materials in a wide range of thicknesses and compositions of building blocks. We discuss the observed features in the low-energy electronic spectra and relate them to the relevant macroscopic properties.

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Anisotropic Magneto-Resistance and Planar Hall Effect in Dual-Gated Topological Insulator Thin Films

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Experimental studies of novel phenomena in three-dimensional (3D) topological insulators (TIs) often require the ability of moving the Fermi level across the Dirac point. Both back gating and top gating techniques have been successfully applied to 3D TI thin films. However, with a single gate, the chemical potential of only one surface can be controlled effectively. Recently, we have succeeded in developing an efficient method for fabricating dual-gated devices on TI thin films grown by molecular beam epitaxy. The method combines (i) the transfer of a high-quality bulk-insulating $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ (BST) thin film grown on sapphire onto a Si/SiO₂ wafer, which serves as a back gate, and (ii) the fabrication of a top gate by using a low-temperature deposition of SiN_x. We demonstrate that the dual gating provides effective control of the chemical potential on the top and bottom surfaces, allowing to move the Fermi level across the Dirac points on both surfaces.

Using the dual-gating technique, we were able to bring the Fermi level into the gap of the insulating BST film, effectively changing the concentration and type of the surface Dirac fermions on both top and bottom surfaces. Measuring the angular dependence of the resistance in the constant magnetic field which is rotated in the plane of the sample, we found a clear anisotropic magneto-resistance (AMR) [$\rho_{xx}(\varphi) \sim \cos^2\varphi$, where φ is the angle between the directions of the current and the magnetic field] and a planar Hall effect (PHE) [$\rho_{yx}(\varphi) \sim \cos\varphi \cdot \sin\varphi$] in our films. It has been known for decades [1] that such MR can be realized in ferromagnetic materials, but it is completely unexpected in non-magnetic BST films. Moreover, the amplitude of MR anisotropy and PHE can be effectively controlled by electrostatic gating. We argue the relevance of this observation to the unique spin-momentum locking in TIs.

This work is done in collaboration with Yoichi Ando, Fan Yang, Satoshi Sasaki, Kouji Segawa, Yasuhide Ohno, and Kazuhiko Matsumoto. The research is supported by JSPS (KAKENHI 25400328), MEXT (Innovative Area “Topological Quantum Phenomena” KAKENHI), AFOSR (AOARD 124038), Inamori Foundation, and the Murata Science Foundation.

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Domain Walls in Junctions of Thin Film Magnets and 3D Topological Insulators

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The spin-transfer torque generated by the surface states of a 3D Topological Insulator (TI) has recently been measured [1] to be larger than for any other spin-transfer torque source measured so far, which encourages the applicability of junctions of thin film magnet and TIs for spintronic based devices. We analytically compute the effective action for the magnetization in this system with an out-of-plane domain wall (DW) equilibrium configuration, at finite density and in the presence of an external electric field. We show that an electronic chiral state appears bounded to the DW carrying 1D equilibrium (at finite density) and out of equilibrium (at non zero electric field) dissipationless currents. We show that in addition the chiral state generates an in-plane hard axis anisotropy term in the direction perpendicular to the DW. We also address whether a Dzyaloshinskii-Moriya (DM) type of interaction is generated, concluding that it is not the case. However we show that the 1D equilibrium current generates a term that resembles the interfacial DM interaction, but with the important difference that it is a first order term in the magnetization.

The equilibrium profile of the DW is computed as a function of the chemical potential, qualitatively reproducing the behavior of recent numerical results [2], and the physical explanation of the effect is shown to lie in the competition of the chiral 1D current and the induced hard axis anisotropy. This is a novel understanding of the physics and only possible with an analytical approach. We also study the current induced motion of the DW, and confirm that the threshold for Walker breakdown is determined by the exchange interaction, as was stated in [3]. However, we show that this is the case even at neutrality, when there is no equilibrium chiral current, due to the induced hard axis anisotropy. At finite chemical potential and/or external electric field we show that this threshold can be further increased by the presence of equilibrium and/or non equilibrium chiral currents. Having an analytic control of the Hamiltonian paves the path for future investigations, for example addressing magnonic propagation and the possible appearance of a TI induced magnonic torque on the DW.

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Chiral degeneracies and Fermi-surface Chern numbers in bcc Fe

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The degeneracies in the spinor bandstructure of bcc Fe are studied from first principles. We find numerous isolated band touchings carrying chiral charges of magnitude one (Weyl points) or two (double-Weyl nodes), as well as nonchiral degeneracy loops. Some degeneracies are located on symmetry lines or planes in the Brillouin zone and others at generic low-symmetry points, realizing all possible scenarios consistent with the magnetic point group. We clarify the general theory relating the chiral band touchings to the Chern numbers of the Fermi sheets enclosing them, and use this approach to determine the Chern numbers on the Fermi surface of bcc Fe. Although most Fermi sheets enclose Weyl nodes, in almost all cases the net enclosed charge vanishes for symmetry reasons, resulting in a vanishing Chern number. The exceptions are two inversion-symmetric electron pockets along the line Δ parallel to the magnetization. Each of them surrounds a single Weyl point, leading to Chern numbers of ± 1 . These small topological pockets contribute a sizable amount to the nonquantized part of the intrinsic anomalous Hall conductivity, proportional to their reciprocal-space separation.

***Ab initio* Study Of Electronic And Magnetic Properties Of Fe-doped Topological Insulators**

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The focus of the present *ab initio* work is on the electronic structure and magnetic properties of Bi₂Se₃ and Bi₂Te₃ topological insulators (TIs) doped with Fe.

So far, contradictory results have been reported for the electronic as well as magnetic properties of TIs doped with magnetic elements. For example, results point to bulk- and surface-doped samples behaving differently. As an example, the opening of the Dirac point was reported only for bulk-doped systems [1,2], while for surface doped systems reports are contradictory [3,4].

Using the multiple scattering Korringa-Kohn-Rostoker (KKR) approximation together with the coherent potential approximation (CPA) for simulating the doping of the TIs, we carry both electronic structure calculations as well as the computation of magnetic ground state properties. Two cases are shown [all reported results correspond to low dopant concentrations (<20%)].

On the one hand we study the surface Fe doping of Bi₂Se₃, where Fe atoms are experimentally found to replace Bi sites [5]. For such a substitutional Fe position the present work predicts a non-collinear magnetic structure, together with an opening of a gap in the Dirac surface state above a certain Fe concentration.

On the other hand, we track the evolution of the aforementioned properties of Fe-doped bulk alloys Bi₂(Se_{1-x}Te_x)₃, from Bi₂Se₃ to Bi₂Te₃ as a step in understanding a possible path in the tuning of induced magnetic properties of TIs.

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Topological phenomena in photonics

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Topologically non-trivial states have been raising a substantial interest in the electronics community because of their novel and unique properties. Similarly, topological states in photonics display an equally diverse range of novel and surprising phenomena. I will present some of our recent work in this area, including a photonic analogue of Quantum Anomalous Hall Effect [1,2], and Weyl points [3]. In addition, we also discuss embedded eigenvalues in photonic crystal systems [4], whose robustness can also be understood as emerging from certain topological properties.

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Artificial graphene under the spotlight: a realisation of the Bernevig-Hughes-Zhang model

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Floquet topological insulators (FTIs) are topological insulators out of equilibrium. An important example is the honeycomb lattice irradiated by circularly polarised light, which exhibits quantum Hall type edge states due to the irradiation [1]. For radiation frequencies larger than the bandwidth of the system, one can average out the perturbation to obtain an effective description. In this quasi-equilibrium limit, one can classify the system as being in a quantum anomalous Hall state, since the circular polarisation of the light breaks time-reversal symmetry.

As the radiation frequency becomes of the order of the bandwidth, the quasi-equilibrium viewpoint breaks down, and the topological behaviour of Floquet systems is poorly understood. This occurs because photon resonances can open additional gaps in the spectrum hosting topological edge states. In the case of irradiated honeycomb lattices, the appearance of these photon resonances can be understood in terms of band inversion [2]. Using the radiation frequency as a parameter, a hierarchy of band inversions occurs. In general, these extra band inversions create additional topological states in the spectrum of the system. We furthermore derive an effective model for the two-photon resonance, which appears when the photon frequency is half the bandwidth. This effective theory turns out to just be the Bernevig-Hughes-Zhang model for band inversion in an equilibrium topological insulator. In this way, a link is established between equilibrium and out-of-equilibrium topological-insulator descriptions.

Furthermore, this reasoning can also be extended to non-trivial geometries like the Moebius band. While a quantum Hall effect is not globally possible on a Moebius band [3], one can locally induce quantum Hall states through the use of domain walls. Taking into account the appearance of hybridisation effects at such domain walls [4], the view of band inversion remains valid even in this case.

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Dirac plasmonics of Topological Insulators

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Recently, a new development in the field of plasmonics has been achieved by means of engineering plasmonic structures in Topological Insulators (TIs). Indeed, their peculiar properties such as 2D intrinsic transport carried out by Dirac fermions, very high surface density ($n \geq 10^{13} \text{ cm}^{-2}$) compared to the typical values for metallic surfaces, backscattering protection and robustness of the topological phase at room T, make them perfect candidates to develop plasmon based technology. We performed a study of plasmonic excitations on topological insulator Bi₂Se₃-based devices in the THz range, using Fourier Transform Infrared spectroscopy. We investigated resonances dispersion in thin film samples patterned with several shapes by means of Electron Beam Lithography. A first study was performed on Bi₂Se₃ micro-ribbon arrays, enabling to trace the energy-momentum dispersion for plasmonic excitations, in good agreement with the relation expected for 2D gases $\omega \propto k^{1/2}$. Most importantly, we found a very good quantitative agreement with that predicted for Dirac plasmons [1]. Then we investigated devices patterned with microring arrays [2], which exhibit two distinct resonances (bonding and antibonding), arising from the hybridization between disk and anti-dot resonances. The measured extinction coefficient has been compared to ab initio analytical model for plasmonic resonances, through a collaboration with the Institute of Photonic Sciences in Barcelona. The comparison gives an impressive agreement, given the fact that the model has no free parameter, thus opening the way for further prediction and tailoring of plasmonic devices in the THz range.

Moreover, we studied the collective electronic excitations' behavior through the quantum phase transition (QPT) from a TI to a conventional band insulator exploiting the plasmonic properties of micro-ribbon arrays of (Bi_{1-x}In_x)₂Se₃. Under the effect of In-Bi substitution, this material undergoes a QPT around $x=0.05$ as recently observed by means of ARPES and time domain spectroscopy. We found that plasmon linewidth undergoes a strong broadening across the transition, mirroring the single particle's one, and thus giving a strong indication of the topological protection of plasmons in the non trivial phase.

Finally, we studied the excitations on Bi₂Se₃ micro-ribbon arrays under the effect of a strong magnetic field (up to 30 T) [3], observing for the first time magnetoplasmons on topological insulators. By analyzing the magnetoplasmon dispersion and the cyclotron resonance as a function of the field, we were able to extract the dynamical mass of Dirac carriers to $m=0.18 \text{ me}$.

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Surface transport on bulk and thin film topological insulators

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Topological insulators (TIs) are guaranteed to reveal metallic and spin-polarized surface states on an insulating bulk. However, this material class suffers often from *intrinsic* defects, e.g. degradation and vacancies, yielding easily dominant bulk transport channels. Moreover, atomic steps, magnetic impurities, edge-edge interaction, etc., can severely alter the properties of these robust edge states. In this talk we will systematically address these aspects by surface transport measurements as a function of the probe spacings, sample temperature, magnetic field, stoichiometry and film thickness.

The issue of bulk defects was first overcome for Bi₂Te₂Se where compensation of defects leads to low bulk conductivity and surface-dominated transport could directly be observed [1]. Here we present latest measurements of surface-dominated conduction on atomically clean surfaces of bulk Bi₂Te₃. Using a four tip STM for nano-scale four point transport measurements with variable contact distance we show that the transport at 30 K is again two-dimensional rather than three-dimensional. The sheet conductivity of $7.9 \times 10^{-4} \Omega^{-1}$ corresponds to a carrier mobility as high as $2000 \text{ cm}^2/\text{Vs}$. First transport measurements across various step configurations indicate that the robust TI-channel is superimposed by a diffusively scattering 2DEG channel.

Besides these bulk materials we have recently started to grow epitaxial TI-films by in-situ co-deposition on Si(111) substrates in order to reduce bulk contributions and to provide the possibility of nanostructuring. The alloy Bi_{1-x}Sb_x is a 3D topological insulator for concentrations between $x=0.04$ and 0.22 [2]. The morphology was controlled by means of low energy electron diffraction. Temperature dependent transport measurements from 10K to 300 K were performed for films of different stoichiometry ranging from $x=0.14$ – 0.22 and thicknesses of 10, 20, 40 and 60 BL (1BL=0.4nm). Moreover, magneto transport measurements up to 4 T were performed in order to determine carrier concentrations, mobilities and scattering times. For instance, a 30 BL film with a concentration of $x=0.18$ was found to have carrier concentrations of $n=1 \cdot 10^{13} \text{ cm}^{-2}$ and $p=2 \cdot 10^{13} \text{ cm}^{-2}$ with mobilities of $\mu_n=2.6 \cdot 10^2 \text{ cm}^2(\text{Vs})^{-1}$ and $\mu_p=1.9 \cdot 10^2 \text{ cm}^2(\text{Vs})^{-1}$. Most strikingly, at low temperatures transport occurs via a metallic surface channel which abruptly diminishes at a critical thickness of 10BL possibly due to edge-edge interaction leading to an opening of the gap at the Dirac point and resulting in a massive Dirac dispersion [3].

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Sum rule constraints on the surface state conductance of topological insulators

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We report on THz and infrared experiments aimed at probing the Drude oscillator strength and the magnitude of the bulk band gap (E_g) of the epitaxially grown, topological insulator $(\text{Bi,Sb})_2\text{Te}_3$. The magnitude of E_g , in conjunction with the model independent oscillator strength f-sum rule, allowed us to establish an upper bound for the Drude weight expected in a typical Dirac like system with linear bands. The model was extended to include hexagonal band warping, and electron hole asymmetry, as is typical in realistic topological insulator systems. The experimentally observed Drude weight is found to be at or below this theoretical upper bound, demonstrating the effectiveness of alloying in eliminating bulk charge carriers. Moreover, Hall effect parameters and the weak anti-localization observed in transport on the same sample support assignment of the low-energy conduction to topological surface states. Complimentary insights in the response of surface states of $(\text{Bi,Sb})_2\text{Te}_3$ were provided by cyclotron resonance and Faraday rotation experiments in THz frequencies¹.

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Mesoscopic Charge Transport Simulations for Topological Insulators

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The discovery of Topological Insulators has sparked strong research interest in topological properties of condensed matter systems, which imply fundamental and unique features and topological phases [1]. These phases can be realized in complex materials of binary and ternary compounds based on heavy elements, which adds significant complication to their investigation. On the other hand, simplified models [2] allow studying basic fundamental issues and are particularly appealing when the material complexity is such that even simple electronic properties require huge effort for the description at the ab initio level.

In our contribution, we show the results of our transport studies that employ the linear-scaling Kubo transport methodology [3], which has been generalized to account for the spin degree of freedom. We simulate charge transport for large samples of Topological Insulators based on the standard model introduced earlier. [2] Special focus is put on varying the sample geometry [4] and investigating the influence of disorder on transport features.

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DRIVEN TOPOLOGICAL INSULATOR QUANTUM DOT: A SPIN-PARTICLE SOURCE (SPPS)

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Abstract

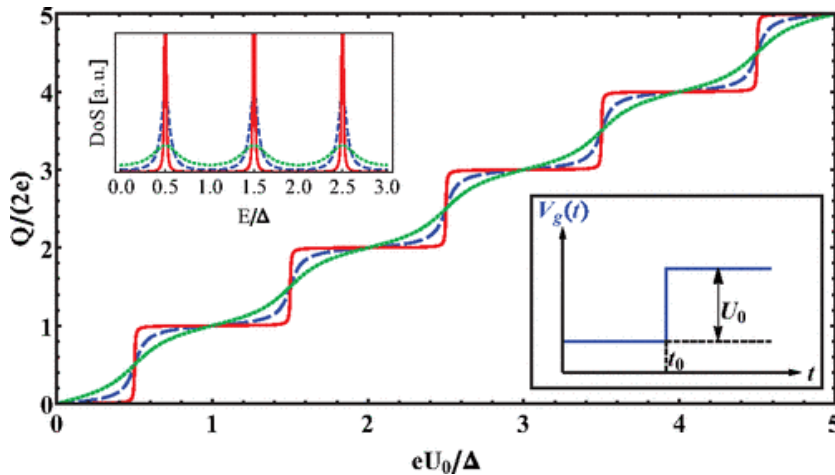
We propose a device that allows for the emission of pairs of spin-polarized electrons into the edge states of a two-dimensional topological insulator [1]. Charge and spin emission is achieved using a periodically driven quantum dot weakly coupled [2] to the edge states of the host topological insulator. We present calculations of the emitted time-dependent charge and spin currents of such a dynamical scatterer using the Floquet scattering matrix approach. Experimental signatures of spin-polarized two-particle emission can be found in noise measurements [3,4]. Here we introduce a new form of noise suppression, named Z_2 anti-bunching. Additionally, we propose a setup in which entanglement of the emitted electrons is generated. This entanglement is based on a post-selection procedure and becomes manifest in a violation of a Clauser-Horne-Shimony-Holt inequality [3].

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Figures

Zero-temperature emitted charge as a function of the height of the driving step and various lines corresponding to different values of the reflection probability of the QPC. Upper inset: The density of states of the QD for various values of $|\lambda_{pb}|$. Lower inset: Model of driving U_0 .



Transport Properties of the Ideal Surface Dirac Cone in the Topological Insulator $\text{Tl}_{1-x}\text{Bi}_{1+x}\text{Se}_2$

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Surface Dirac fermion system of the three-dimensional (3D) topological insulators exhibits a spin-momentum locked electronic state, and the system is understood as a new stage of novel electric- and spin-transport [1]. A number of new topological insulators have been discovered for the past few years. However, most of them turned out to exhibit bulk metallic conduction and the novel surface transport phenomena were hidden in the bulk conduction.

TlBiSe_2 is not only a 3D topological insulator exhibiting a large bulk band gap, but also reported as a bulk metal [1]. Recently, considerable amount of electron doping due to the sample defect was revealed, and by controlling the defect bulk-insulating state was realized [2]. This is the first demonstration other than the Bi_2Se_3 -based topological insulators, and the achievement opens the new stage of researches for the novel surface transport. More importantly, the surface Dirac cone exhibits a simple structure, i.e., the in-gap Dirac point and a small in-plane distortion. These facts indicate that the bulk-insulating TlBiSe_2 is the ideal stage for studies of surface transport.

In this presentation we report the electric transport properties of the TlBiSe_2 of both bulk insulating and bulk metallic samples. The two-dimensional Shubnikov-de Haas oscillations in a bulk-insulating sample were observed. Landau level-fan diagram of the oscillation showed the π Berry phase (see Figure 1), and the fact indicated that the oscillations were originated from the surface Dirac fermions. Mobility of both surface and bulk were determined, and compared with each other. We present our recent data and discuss scattering mechanisms.

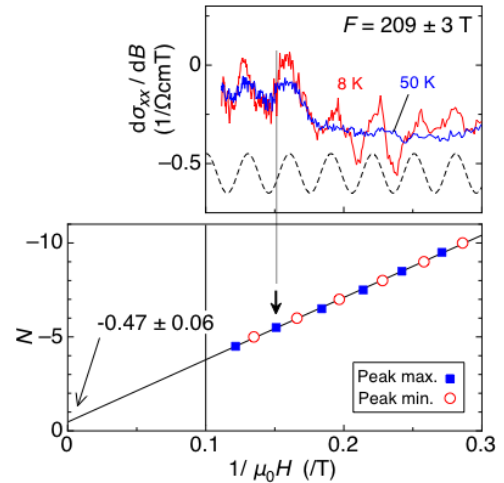


Figure 1: Surface Shubnikov-de Haas oscillation, and the Landau level-fan diagram exhibiting π Berry phase. F is the frequency [3].

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Ultrafast Electron and Lattice Dynamics of a Topological Insulator

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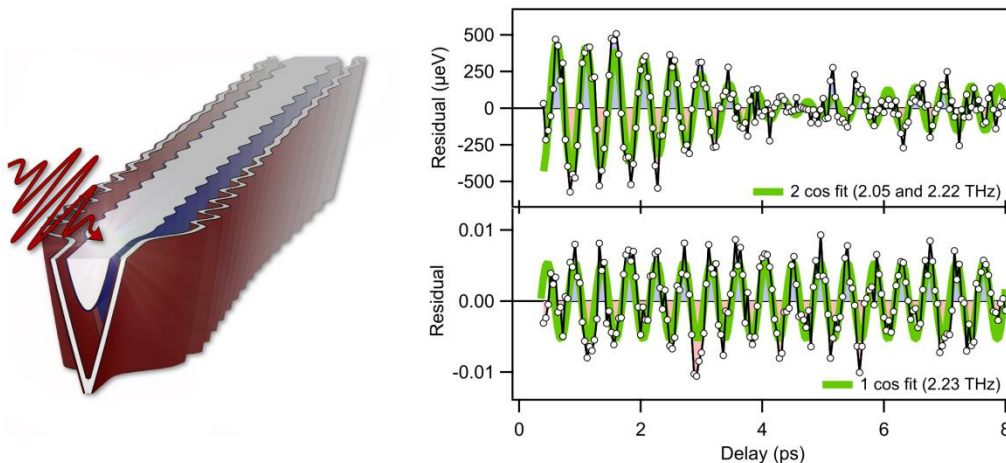
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Topological insulators have a rich electronic structure characterized by the coexistence of insulating bulk states with robust metallic surface states. Understanding the interplay of these electronic states, and their interaction with the crystal lattice, is a prerequisite for their technological application. Here we use time- and angle- resolved photoemission spectroscopy (trARPES) to study the transient response of the topological insulator Bi₂Se₃ upon ultrafast photoexcitation. Our results fall into three categories: (1) By two-photon photoemission processes, we study the unoccupied electronic structure and resolve optical transitions into a second topological surface state [1]. (2) By studying the electron relaxation dynamics, we identify the dominant scattering channels including interband surface-to-bulk scattering as well as intraband electron-phonon scattering [2]. The temperature-dependence of the latter is measured and interpreted with a microscopic model of the scattering processes [3]. (3) With sufficiently intense excitation, we drive coherent lattice motion which results in oscillatory modulations of both the bulk and surface bands. We find an additional frequency in the surface as compared to the bulk, which we interpret as a softening of the phonon near the crystal surface [4]. Our results shed new light on the structure of electronic states in topological insulators and help unveil their dominant scattering mechanisms.



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Electron-Phonon Interaction in Surface States of Topological Insulators from First Principles

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The existence of metallic 2D surface states with a Dirac-like dispersion and a peculiar spin texture is one of the outstanding properties of 3D topological insulators. While this state is topologically protected against time-reversal invariant scattering, transport properties are influenced by many-body interactions. In particular, a large electron-phonon interaction could be a limiting factor for applications at elevated temperatures [1]. Previous investigations of the electron-phonon coupling with various experimental probes remained inconclusive as the derived coupling strengths for the 2D surface states exhibited large variations ranging from <0.1 to 3 [2].

Here we present a *first principles* investigation of the electron-phonon interaction and self-energy of the surface states of a topological insulator, using Bi_2Se_3 as the prime example. It is based on a self-consistent calculation of both vibrational properties and screened electron-phonon vertices for periodic slab geometries within density-functional perturbation theory including spin-orbit interaction [3]. We discuss the various challenges faced by this approach. In particular, the rather deep penetration of the surface state forces the use of rather thick films to properly represent the surface, while the small momentum range of both electronic and phononic states relevant for the coupling requires a highly accurate evaluation of the long-wavelength screening properties. We find that the coupling strength exhibits a significant dependence on the binding energy, following essentially the available electronic phase space. We further investigate the variation of the coupling with doping to mimic typical experimental conditions.

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Samarium hexaboride: a trivial surface conductor

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The historically first mixed-valence compound and first Kondo insulator SmB₆ features a low-temperature resistivity which has remained unexplained for over three decades. Recent predictions as the first topological insulator caused by electron correlation have been supported by a large number of angle-resolved photoemission studies. By proper distinction of Sm and B terminated samples we demonstrate that the existence of surface states (at Γ and X) is independent of the termination. Secondly, we show that both types of surface states appear massive, most clearly the one at the zone center which develops a Rashba spin splitting for B termination excluding an odd number of Dirac cones and topological insulator behavior. It is shown that the metallic surface at low temperature is due to a surface shift of the 4f and a reduced f-d hybridization at the surface which keeps the surface state at X metallic.

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High-throughput search of novel topological materials

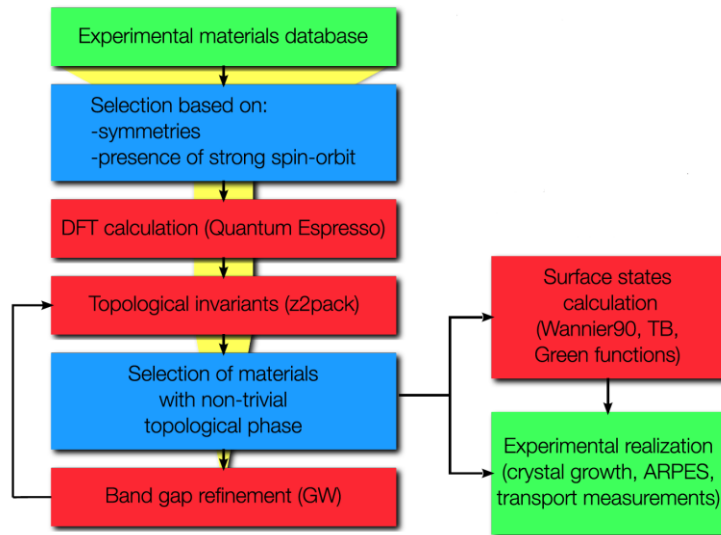
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A large number of different topological electronic phases that can be realized in materials have been predicted recently. While many strong Z_2 topological insulators have been found within the family of layered bismuth and antimony chalcogenides, solid experimental confirmations of materials realizing other topological phases, such as the weak Z_2 topological insulators, topological crystalline insulators, Dirac and Weyl semimetals, are still very scarce. We have developed a methodology for identifying materials hosting various topological phases among known compounds. Our approach is based on the automated high-throughput screening of online databases of experimental crystallographic structures. Initial sampling is performed using simple criteria such as the size of band gap, the strength of spin-orbit coupling and crystallographic space group. The topological invariants of materials within the sample are computed from first principles using the z2pack approach [1,2]. Candidate materials hosting topological phases are further scrutinized by refining the band gap and band ordering by means of calculations employing of the GW approximation. Here, we discuss various aspects of performing such high-throughput screening and present first predictions successfully confirmed by experiments [3].



We acknowledge support from the Swiss NSF (grant No. PP00P2_133552), ERC project “TopoMat” (grant No. 306504) and NCCR-MARVEL.

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Plasmons in topological insulators: from basic research to technological application in THz photodetection

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Topological surface states could find important applications in the field of plasmonics and plasma-wave photodetection. Despite this promising prospect, their potential in this area is hitherto largely unexplored. Recent theoretical works indicate that the surface of topological insulators can support collective electronic excitations of electrons in SS forming the Dirac cone in the THz range ^{1, 2}. The low energy of the Dirac plasmons makes possible their usage for the realization of THz photodetectors to be used, for example, in homeland security.

From the experimental side, optical techniques have been used to investigate plasmon modes of thin films ³ and nanoribbons ⁴ of Bi₂Se₃ at $q \sim 0$. The Dirac plasmon has been observed in Bi₂Se₃ nanoribbons ⁴, while the bulk plasmon has been reported in thin films. However, optical techniques do not allow investigating the momentum-dependence of plasmonic excitations and, thus, the nature and the dispersion of low-energy collective excitations in TI in an extended q -range is hitherto unexplored.

This talk is divided into two parts. In the first one, I will present a study on the dispersion relation of plasmonic modes in topological insulators, while in the second part I will show an application of THz plasmons in topological insulators.

Firstly, I will report on the momentum-resolved investigation of plasmonic excitations of Bi₂Se₃(0001) by means of high-resolution electron energy loss spectroscopy (HREELS), which allows probing an extended momentum range. At a small parallel momentum transfer $q_{||}$, the loss spectrum shows a distinctive feature peaked at 104 meV. Such mode slightly disperses with $q_{||}$. The behavior of its intensity as a function of primary energy and scattering angle allowed us to identify it as a surface plasmon. At larger momenta ($q_{||} > 0.04 \text{ \AA}^{-1}$), an additional peak, attributed to the Dirac plasmon, becomes clearly defined in the loss spectrum. Momentum-resolved loss spectra evidenced the mutual interaction between surface plasmon and Dirac plasmon of Bi₂Se₃. The proposed theoretical model accounting for the coexistence of three-dimensional doping electrons and two-dimensional Dirac fermions well reproduces the experimental observations.

In the second part of this talk, I will also show that thin flakes of Bi₂Se₃ or Bi₂Te_{2.2}Se_{0.8} topological insulators can be used for as active channels in room-temperature THz detectors based on antenna coupled TI-based field-effect transistors (FET), exploiting the plasma-wave photodetection mechanism. A FET hosting a 2D electron gas can act as a cavity for plasma waves (collective density oscillations) and thus photodetection is possible through the generation of a finite dc voltage in response to an oscillating radiation field. The reported performances allow exploiting the devised technology in realistic settings for large-area, fast imaging of macroscopic samples, promising superb impacts of topological insulators on photonic applications across the fascinating THz region of the electromagnetic spectrum.

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Optoelectronic control and characterization of surface state transport in bismuth-based topological insulators

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In principle, bismuth-based topological insulators (TIs), such as Bi_2Te_3 , Bi_2Se_3 or BiSbTe_3 allow realizing surface dominated transport at room temperature due to bulk band gaps up to 0.3 eV. One major challenge is the competing bulk conduction at room temperature.

On the one hand, we show that surface currents in Bi_2Se_3 can be controlled by circularly polarized light on a picosecond timescale with a fidelity near unity even at room temperature (Fig. 1).[1] We reveal the temporal separation of ultrafast helicity-dependent surface currents from photo-induced thermoelectric and drift currents in the bulk.

On the other hand, molecular beam epitaxy growth of TI films on SrTiO_3 substrates allows substantially reducing residual bulk conduction. We locally probe the electronic transport of TI circuits on SrTiO_3 by photocurrent spectroscopy.[2,3] On a micrometer scale, we find that long range potential fluctuations with an amplitude of several meV dominate the transport (Fig. 2). We demonstrate that these potential fluctuations occur predominantly at the topological insulator/substrate interface. These findings may have implications for optimizing the growth of thin topological films as well as for the interpretation of linear magneto-resistance data in terms of electrostatic disorder.

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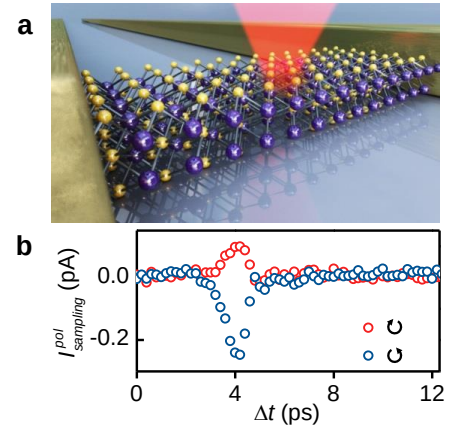


Fig. 1 (a) and (b) A circularly polarized laser pulse controls ultrafast surface currents in Bi_2Se_3 .

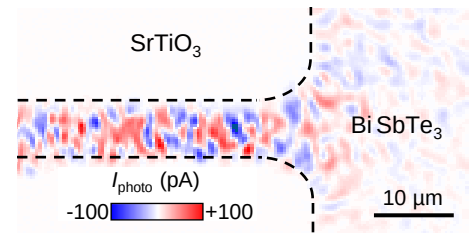


Fig. 2 Local photocurrent spectroscopy reveals potential fluctuations in TI thin films on SrTiO_3 .

Terahertz Radiation Induced Trigonal Photocurrents in $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ Three Dimensional Topological Insulators

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The electronic properties of Dirac fermions in three dimensional (3D) topological insulators (TI) are in the focus of present research. Their study at room temperature is challenging and often hinder by a large residual bulk charge carrier density. Recently we demonstrated that an access to the surface states transport in $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ at room temperature becomes possible studying nonlinear high frequency transport [1].

Here we show that by exciting the $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ samples with terahertz (THz) radiation two photocurrents can be induced, namely the photogalvanic effect and the photon drag effect. These photocurrents are formed due to the trigonal symmetry of the surface states. While the photogalvanic effect is caused by asymmetric scattering of Dirac fermions driven back and forth in the exciting *ac* THz electric field, the photon drag effect is caused by the light momentum transfer to charged carriers. We show that at normal incidence the photocurrent is dominated by the photogalvanic effect, which is only allowed in the non-centrosymmetric surface states. A careful analysis of the frequency dependence shows that the photocurrent is formed due to Drude absorption and allows one the estimation of the scattering times at room temperature. However, at oblique incidence the photogalvanic effect diminishes and the photocurrent formation can be dominated by the photon drag effect. A distinction between both effects becomes possible due to the different behavior on the angle of incidence: while the trigonal photogalvanic effect is decreasing, the trigonal photon drag effect, being zero at normal incidence, increases with the angle of incidence. The latter is caused by increasing out-of-plane component of the radiation electric field. Moreover, by only changing the exciting THz frequency the main contribution to the total photocurrent can be changed. This frequency behavior provides additional information on the light matter interaction in TIs. All presented results are in good agreement with a developed microscopic theory of trigonal photocurrents in 3D TI at room temperature.

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Cyclotron Resonance Induced Photocurrents in HgTe 3D TIs

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Strained mercury telluride films of proper thickness belong to the group of three dimensional topological insulators [1] and are in the focus of recent research. Due to strain a gap opens, in the otherwise gapless bulk of HgTe, resulting in a insulating bulk and conducting surface states. This fact, together with the high quality of the material, allows one to investigate the electronic transport in surface states only [1,2]. Here, we report on the observation of the cyclotron resonance assisted photocurrents in the surface states of HgTe based topological insulators [3]. To study the cyclotron resonance in 80 nm HgTe films, we applied a continuous wave terahertz laser radiation. The photocurrent data, accompanied by transport experiments and measurement of radiation transmission, prove that the resonant photocurrent is generated in the topologically protected top and bottom surface states. We demonstrate that studying these responses in gated samples, provides a sensitive method to probe the cyclotron masses of two dimensional Dirac top and bottom surface states as a function of the Fermi energy. For large gate voltages we detected an additional CR at a higher magnetic field, which is caused by bulk carriers, and corresponds to a mass about two times larger than that obtained for the surface states. To analyze the resonances, we calculated the band structure by $k \cdot p$ method and obtained cyclotron masses of the surface states and the bulk states of 80nm HgTe films, which fit well to the experimental data. Based on these data we developed a microscopic theory of the resonance photocurrent and show that the effect emerges due to an asymmetric scattering of carriers in the momentum space resulting in a fully spin polarized dc electric current.

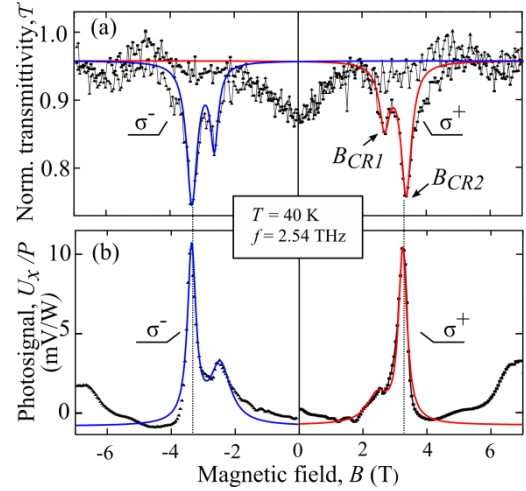


Fig. 1: (a) Cyclotron resonance response of the top and bottom surface states (B_{CR1} and B_{CR2}) measured by radiation transmission and photocurrent.

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Prediction and design of quantum spin Hall and quantum anomalous Hall phases from first principles

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The realization of dissipationless spin- and charge transport in two-dimensional (2D) topological insulators (TIs) requires the optimization of material parameters, e.g., the stabilization of the 2D material on a substrate maintaining a suitable size and position of the band-gap, a reasonable localization of the edge states or, for the Chern insulators, the introduction of a proper exchange splitting in the material. Density functional theory is a powerful tool to predict these properties and give new ideas to design functional materials experimentally. In this contribution, the focus will be on functionalized variants of Bi bilayers, but also 2D TIs that are obtained as thin films of their three-dimensional counterparts.

While contact with substrates often leads to doping that shifts the band-gap away from the Fermi level [1], hydrogenation can minimize the interactions so that a Bi layer can be stabilized on a MoS₂ substrate maintaining its insulating properties [2]. The functionalization also allows to introduce magnetism in the layer and to realize the so-called valley-polarized quantum anomalous Hall effect. This will be compared to other strategies proposed to drive a system from the quantum spin Hall to the quantum anomalous Hall regime, e.g., by proximity of a magnetic substrate [3]. Finally, the prospects of 2D topological crystalline insulators and their practical realization will be shortly discussed.

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Hall viscosity from elastic gauge fields in Weyl crystals

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We investigate the presence and physical implications of elastic gauge fields in a large set of crystalline materials with non trivial topology in two and three dimensions. We demonstrate that, in these "Weyl crystals", Hall conductivity implies Hall viscosity. The new mechanism generates a Hall viscosity orders of magnitude bigger than the previously studied response.

Topological Index For Periodically Driven Time-Reversal Invariant 2D Systems

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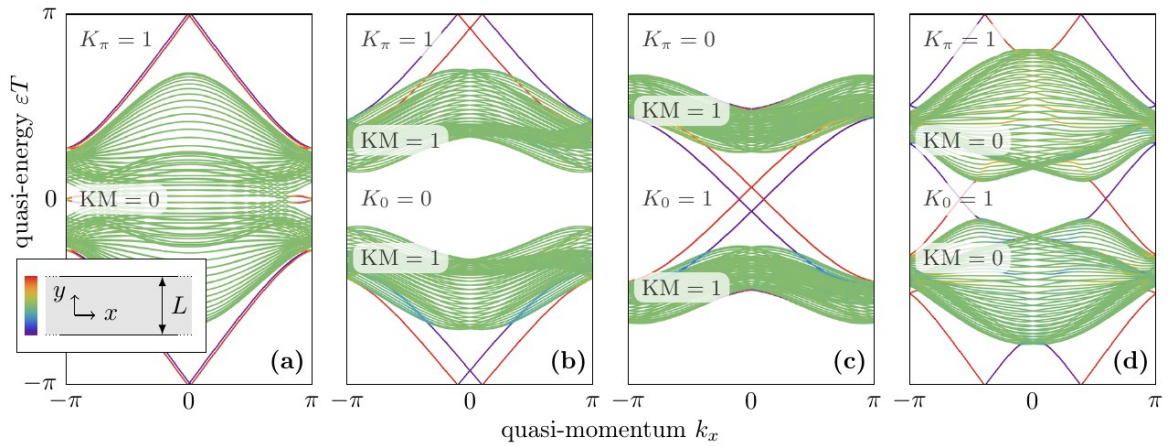
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A characteristic feature of gapped systems is that they have no low energy excitations. Yet, the interface between two gapped systems may host some kind of protected low-energy excitations, which are impossible to get rid of. This arises from the non-trivial topology of the ground state of the system, usually characterized by a topological invariant. Such *topological phases* were first discovered in condensed matter systems, with the quantum Hall Effect. The seminal paper by Kane and Mele [1] made apparent the importance of symmetries such as time-reversal in the appearance of the so-called symmetry protected topological phases.

With the goal of achieving a better control of topological phase transitions in electronic systems, it was proposed to produce out-of-equilibrium (but stationary) topological phases through a periodic driving, such as the application of light [2]. Yet, out-of-equilibrium phases display richer topological features than equilibrium phases and a new framework to fully describe the topological properties of the unitary evolution of a two-dimensional periodically driven system without specific symmetry was developed [3].

We define a new $\mathbb{Z}_2$ -valued index, denoted by K , to characterize the topological properties of periodically driven two dimensional crystals when the time-reversal symmetry is enforced [4]. This index is associated with a spectral gap of the evolution operator over one period of time. When two such gaps are present, the Kane-Mele index of the band between the gaps is recovered as the difference of the gap indices. This also leads to an expression for the Kane-Mele invariant in terms of the Wess-Zumino amplitude.



Quasi-energy spectra of a ribbon subjected to a time-reversal periodic driving. The value of the new K index predict the existence of the edge states (in red/blue) in the gaps.

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Field Theory of Proximity-Induced Magnetism in Topological Insulators

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Topological insulators are characterized by symmetry-protected gapless boundary states. Particularly interesting are the three-dimensional topological insulators, whose electromagnetic response features a topological magnetoelectric effect which is closely related to the so-called chiral anomaly in relativistic quantum field theories. In the context of solid state physics the chiral anomaly arises as a second-quantized version of the Berry phase induced by the electromagnetic response of topological insulators. This property plays an important role in heterostructures involving both topological insulators and magnetic materials. In this talk we will consider theoretical and experimental aspects of bilayer and trilayer structures of the form FM/TI and FM/TI/FM from the point of view of quantum-field theoretic anomalies. The paradigmatic experimental example to be discussed within a field-theoretical approach is one where FM=EuS and TI=Bi₂Se₃, as there are recent experiments available with structures involving these two materials, including a recent experimental demonstration of room temperature proximity-induced ferromagnetism in an EuS/Bi₂Se₃ bilayer system and on how it can be understood theoretically.

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Relativistic GW Calculations for Topological Insulators: Quasiparticle Effects on the Bulk and Surface States.

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Most theoretical studies of topological insulators are nowadays based on model Hamiltonians, parameter-dependent tight-binding descriptions, and density functional theory employing either the local-density (LDA) or generalized gradient approximation. But recently, many-body calculations within the GW approximation were attracting much attention in the study of these materials. Within the all-electron FLAPW formalism and taking fully into account spin-orbit coupling (SOC) [1], we have performed LDA and GW calculations for the topological insulators Bi_2Se_3 , Bi_2Te_3 and Sb_2Te_3 [2], as well as for the ternary compound of the same family $\text{Bi}_2\text{Te}_2\text{Se}$. We will present a comparison of the calculations to angle-resolved photoemission spectroscopy (ARPES) data [3]. We find that the GW corrected bands agree much better with experiment than the LDA bands.

We will also present an implementation of the quasiparticle self-consistent (QS) GW method where the SOC is fully taken into account in each iteration rather than being added a posteriori. We have applied this method to the semimetal Bi and found a very good qualitative and quantitative description of the electronic band structure. Therefore, we have used this approach to analyze the effect of strain on the topological properties of bulk Bi. Whereas LDA predicts that an impractical stress is needed for a trivial-to-topological transition, QSGW shows that bulk Bi becomes a topological semimetal already under very small stress [4].

GW and QSGW calculations for low-dimensional systems are still computationally very demanding. Therefore, in order to study the topological surface states with an approach based on GW, we use Wannier functions to construct a Hamiltonian that reproduces the many-body band structure of the bulk system. This Hamiltonian can then be used to construct a slab Hamiltonian. We will use this approach to discuss the effect of quasiparticle corrections on the surface states of some of the examples mentioned above and on the interaction between bulk and surface states.

Funding has been provided by the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

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Atomic and electronic structure of the pristine and adsorbate covered Bi₂Se₃ (0001) surface

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Topological insulators (TI) represent an unusual state of matter. While they are insulators in the bulk they are metals at the surface characterized by a linearly dispersing topologically protected surface state ("Dirac cone") bridging the bulk band gap. Owing to its large band gap, Bi₂Se₃ is an archetype TI and tremendous interest has emerged to investigate the electronic structure and transport properties of its pristine and adsorbate covered (0001) surface. The latter is motivated by the search for new exotic quantum effects and the question whether the topological state is robust against adsorption of magnetic and non-magnetic adsorbates. By contrast, quantitative information concerning the atomically resolved geometric surface structure is surprisingly scarce. This talk gives an overview over recent progress in the analysis of the atomic structure of the pristine and adsorbate covered Bi₂Se₃ (0001) surface as well as its relation to the electronic properties using surface x-ray diffraction (SXRD), x-ray absorption spectroscopy (XAFS), scanning tunneling microscopy and angular resolved photoemission spectroscopy experiments.

Using SXRD it was shown that trace amounts of carbon, which may not be detected by Auger electron spectroscopy induce an expansion of the top layer (Se-Bi) spacing by several percent which goes in parallel with an upward shift of the Dirac point (DP) by 40 meV [1,2]. Upon adsorption of submonolayer amounts of iron and noble metals like gold and silver at 160 K sample temperature SXRD and XAFS measurements indicate the substitution of bismuth atoms. ARPES measurements for Au/Bi₂Se₃(0001) show an opening of the gap at the DP. By contrast, for deposition of cesium up to a maximum film thickness of 0.3 monolayers, substitution of top selenium atoms was observed which is related to the formation of Rashba split two-dimensional metallic states. No incorporation of cesium atoms into the van der Waals gap is observed. The results are discussed in the context of ab-initio calculations.

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Tunable Dirac electron and hole self-doping of topological insulators induced by stacking defects

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Via density functional theory based calculations we show that self-doping of the surface Dirac cones in three-dimensional Bi_2X_3 ($\text{X}=\text{Se}, \text{Te}$) topological insulators can be tuned by controlling the sequence of stacking defects in the crystal. Twin boundaries inside the Bi_2X_3 bulk drive either n - or p -type self-doping of the (0001) topological surface states, depending on the precise orientation of the twin. The surface doping may achieve values up to 300 meV and can be controlled by the number of defects and their relative position with respect to the surface. Its origin relies on the spontaneous polarization generated by the dipole moments associated with the lattice defects. Our findings open the route to the fabrication of Bi_2X_3 surfaces with tailored surface charge and spin densities in the absence of external electric fields. In addition, in a thin film geometry two-dimensional electron and hole Dirac gases with the same spin-helicity coexist at opposite surfaces.

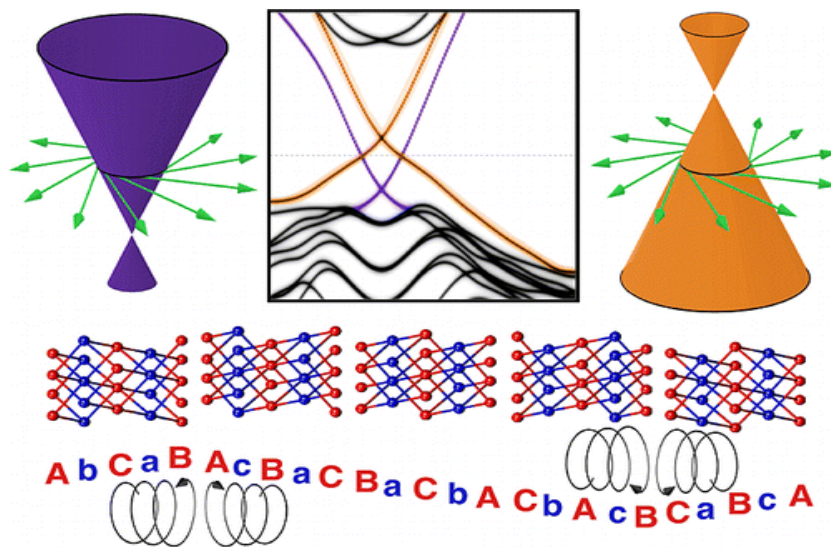


Figure: Band structure of a 6 Quintuple Layer thick Bi_2Se_3 slab including two twin boundaries. Topological surface state (TSS) at the bottom surface (purple) shows n -doping, whereas the TSS at the top surface (orange) shows p -doping. The spin texture of the helical TSSs (spin-momentum locked) is shown by the arrows in the respective Dirac cones.

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Topological Crystalline Insulator in a new Bi semiconducting phase

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In this contribution, by means of structure prediction calculations, we report a new semiconducting phase of Bi with a bulk band gap of 160 meV which is a topological crystalline insulator with mirror Chern number -2 and trivial Z₂ invariant. This Bi lattice is therefore a topological crystalline insulator, but not a strong topological insulator. It displays 2 mirror planes and the band structure shows two non-trivial surface states at the {001}-surface at each of the mirror lines. Because topological protection comes from the crystal symmetry, magnetic impurities or magnetic fields perpendicular to the mirror plane are not expected to open a gap in the surface states in topological crystalline insulators. Instead, the gap can be open with a perpendicular electric field. Considering the outstanding properties of Bi and the fact that its surface states are topologically protected, this discovery opens a new gate to topological electronics and spintronics applications.

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In-situ Spectroscopy of Intrinsic Bi₂Te₃ Topological Insulator Thin Films And Impact of Extrinsic Defects

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Bismuth telluride (Bi₂Te₃) is one of the 3D topological insulator (TI) materials that have received a considerable amount of attention as potential candidates for room temperature spintronics and quantum computational devices[1]. However, despite significant progress in TI material preparation, growing high-quality TI materials for transport experiments is still a major challenge. Often, bulk carrier conduction complicates direct observation of surface effects in transport measurements.

Molecular beam epitaxy (MBE) is an established method for growing high-quality crystalline thin films of Bi₂Te₃ with surface-dominated conduction [2-4]. Nevertheless, to date it is not well understood how in-vacuo storage and extrinsic defects affect surface and bulk states of Bi₂Te₃ thin films.

In this work, we first focus on optimizing our growth procedure in order to realize bulk insulating films. Our combined in-situ x-ray photoemission spectroscopy and in-situ scanning tunnelling spectroscopy study of molecular beam epitaxy grown Bi₂Te₃ on Al₂O₃(0001) reveal high quality stoichiometric thin films and topological surface states without a contribution from the bulk bands at the Fermi energy[5]. By analysing conductance spectra of our Bi₂Te₃ films, we find that the tunnelling differential conductance is well described by that of a warped Dirac cone, including an additional ‘kink’ term in the Γ –M direction[5]. Investigating the effect of pure oxygen exposure at atmospheric pressure; and then the effect of ex-situ contamination in air, we observe that the surface morphology and electronic band structure of our Bi₂Te₃ films are not affected by in-vacuo storage and exposure to oxygen; whereas major changes are observed when exposed to ambient conditions[5]. Using a recent helical magnetoresistance model[6], magnetotransport data of a 70 nm film of Bi₂Te₃ are fitted. We observe that the obtained spin-orbit energy for the film is slightly higher than for the thicker flake of Bi₂Te₃, highlighting that our films are free from intrinsic defects as also seen in STM topography of atomically smooth Bi₂Te₃ surface. Our study help define a pathway towards intrinsic topological devices.

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Tuning the Fermi energy to the Dirac point in the ternary topological insulator $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$

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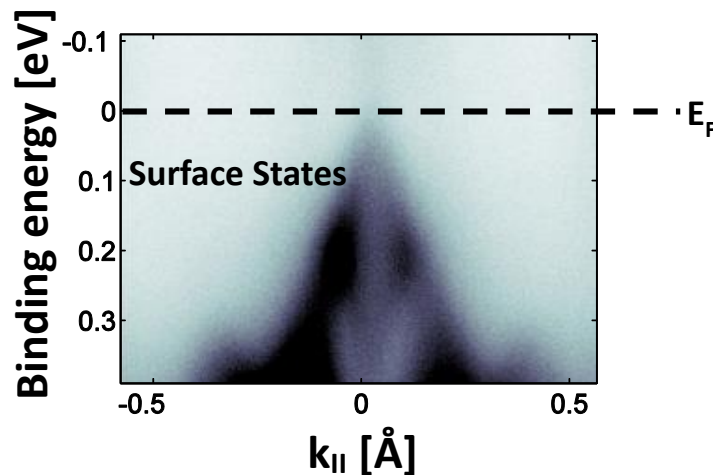
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A topological insulator (TI) has a bulk energy gap but conducting helical surface states. In order to make use of these states, e.g. in transport devices or for creating exotic quasiparticles like Majorana Fermions, one has to tune the Fermi energy (E_F) close to the Dirac point (E_D) within the band gap.

However, currently used TI materials e.g. Bi_2Te_3 and Sb_2Te_3 have major drawbacks. For Bi_2Te_3 , E_D is buried in the bulk valence band (BVB) and E_F is located in the bulk conduction band (BCB) [1]. Whereas with Sb_2Te_3 , E_D is in the bulk energy gap and E_F is located in the BVB [1]. Mixing the two compounds leads to a ternary system $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ where charge compensation is achieved and the position of E_D can be tuned [2]. So far no group has grown and measured a ternary topological insulator, with a Dirac point located on the Fermi niveau and no BVBs contributions [2-5].

We were able to synthesize $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ thin films for $0.95 < x < 0.96$ by molecular beam epitaxy (MBE), transferred in-situ in ultrahigh vacuum from the MBE system to the photoemission setup. Angle resolved photoemission spectroscopy (ARPES) shows that E_F and E_D are congruent and no bulk bands intersect E_F .



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Chaotic Quantum Dots with Tunnel barrier – Scattering from a Majorana bound state

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We calculate the joint distribution $P(S,Q)$ of the scattering matrix S and time-delay matrix $Q=-i\hbar S^\dagger dS/dE$ of a chaotic quantum dot coupled by point contacts to metal electrodes. While S and Q are statistically independent for ballistic coupling, they become correlated for tunnel coupling. We relate the ensemble averages of Q and S and thereby obtain the average density of states at the Fermi level. We apply this to a calculation of the effect of a tunnel barrier on the Majorana resonance in a topological superconductor. We find that the presence of a Majorana bound state is hidden in the density of states and in the thermal conductance if even a single scattering channel has unit tunnel probability. The electrical conductance remains sensitive to the appearance of a Majorana bound state, and we calculate the variation of the average conductance through a topological phase transition.

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The Effect Of Strain On The Two-Dimensional Topological Insulator HgTe

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In the past years, HgTe quantum wells have been used extensively to study the magnetotransport signature of two-dimensional topological insulators, namely the quantum spin Hall effect. It has been shown that the band structure of those systems strongly depends on the thickness of the quantum well, and that, in particular, the topology changes from trivial to nontrivial at a critical thickness of 6.3 nm [1].

As an additional degree of freedom, the influence of strain on the band structure is investigated in this work. By growing CdTe-Cd_{0.5}Zn_{0.5}Te superlattices on GaAs as virtual substrates in a combination of molecular beam epitaxy and self-limiting atomic layer epitaxy, we are able to precisely tune its effective lattice constant (figure 1). The strain of the HgTe quantum well layer grown subsequently can be varied from tensile to compressive, which modifies the shape of the valence band (figure 2).

Depending on strain, temperature dependent transport measurements on nominally identical, wide quantum wells ($d = 17$ nm) reveal either features of topological insulators or semimetals, and the bandgap values obtained from fitting agree nicely with band structure calculations. Further experiments focus on the correlation between the magnitude of the inverted bandgap and stability of the quantum spin Hall edge states, and may help to understand the backscattering mechanisms in these helical channels.

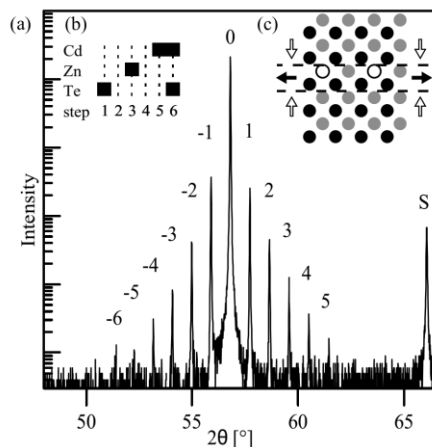


Figure 1 (a) HRXRD-scan of a typical CT-CZT superlattice. (b) shutter sequence of one growth cycle. (c) resulting layer of one growth cycle

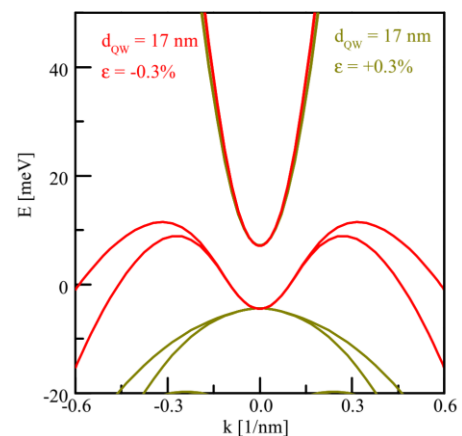


Figure 2 influence of strain on the band structure of a HgTe quantum well with thickness $d = 17$ nm.

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Influence of the surface reorganization on the spin electronic structure of the Dirac cone of topological insulators

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The main features of 3D Topological Insulators (TIs) are the spin-polarized Topological surface states with the Dirac-cone like dispersion. Similar to that, 2D topological insulators, such as bilayer of Bi, are characterized by 1D edge states. The intriguing phenomenon is associated with the coexistence of 1D and 2D edge states, i.e. contact of 2D with 3D topological insulators. A theoretical and experimental studies of single-bilayer Bi(111) ultrathin film on 3D TIs were recently performed, see for example [1,2], showing the presence of both types of topological states.

Another interesting problem is a quantum-tunneling modulation of the topological surface states in thin films of TIs. It is well known that compounds Bi-Te-Se, being 3D TIs, are composed of 5 layer blocks (QLs). If the sample consists of few QLs states from opposite surfaces interfere and destroy the unique structure of the Dirac cone.

In this work we experimentally demonstrate that the surface QLs of 3D TIs $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ can transform to another composition by brief anneal of the sample. By means of STM, XPS and ARPES we show a formation of a Bi-bilayer under 1st surface QL. Such a structure allows us to study a system 3D TI - 2D TI - 1 QL of Bi-Te-Se, where the latter is 3D TI in quantum-tunneling limit. By means of ARPES with spin resolution we investigated the details of the spin and electronic structure of the formed Dirac-like states, their hybridization and a formation of a local gaps.

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Missing Shapiro Step in Bi₂Se₃ Josephson Junction

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Josephson junction made by contacting a 3D topological insulator (TI) with conventional superconducting electrodes may harbor zero-energy Andreev bound states, that is, Majorana Fermions [1]. Theory predicts that a way to unveil the presence of those Majorana bound states consists in irradiating a Josephson junction with a rf field to induce Shapiro steps in the IV characteristics. In the topological phase, the presence of the Majorana mode should lead to a suppression of all odd Shapiro steps [2]. Here we present experimental data showing the disappearance of only the first Shapiro step in Josephson junctions made on Bi₂Se₃ flakes. Whereas some missing Shapiro steps at high rf frequency can be accounted for by trivial hysteresis effects, we observe at low rf frequency a disappearance of the first step on both switching and retrapping currents. Our observations resemble those obtained on InSb nanowires [3] and HgTe [4] 3D topological insulator. However the fact that our Bi₂Se₃ samples shows metallic character with bulk conduction casts doubt about the Majorana origin of the missing first Shapiro step.

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First-principles approach to microscopic understanding of quasiparticle interference on the strong topological insulator Bi₂Te₃

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Quasiparticle interference (QPI) patterns, typically measured by scanning tunneling microscopy (STM), give the possibility to experimentally access the scattering phenomena of electrons near surfaces [1]. This access is gained by comparing the Fourier transform of the QPI images with the knowledge of the Fermi surface of the system using the joint density of states (JDOS) [1,2]. The JDOS is the self-convolution of the Fermi surface, known e.g. from angle resolved photoemission or density functional theory calculations, that gives access to possible scattering vectors which determine the QPI patterns around impurities. It is usually extended by the scattering matrix $M(\vec{k}, \vec{k} + \vec{q})$ to get the spin-dependent scattering probability (SSP) [1] which is calculated from the spectral function in $\vec{k}$ -space $A(E, \vec{k})$, i.e. the constant energy contour $E(\vec{k})$, via

$$SSP(E, \vec{q}) = \int A(E, \vec{k}) M(\vec{k}, \vec{k} + \vec{q}) A(E, \vec{k} + \vec{q}) d^2k. \quad (1)$$

Typically the scattering matrix $M(\vec{k}, \vec{k} + \vec{q})$ is approximated by modeling the spin structure of the surface state with $M(\vec{k}, \vec{k} + \vec{q}) = (1 + \cos \theta_{\vec{q}})/2$, where $\theta_{\vec{q}}$ is the angle between $\vec{k}$ and $\vec{k} + \vec{q}$ [2]. For a correct interpretation of the scattering phenomena in systems with broken structural inversion symmetry, it is very important to take the spin into account [3]. This is especially true in topological insulators with their extraordinary, helical surface states. Here the spin momentum locking leads to protection against backscattering, if time-reversal symmetry is present.

In this contribution we go beyond the usual approximations and assumptions made in the calculations of the JDOS [1,2] and include the microscopic scattering probabilities for scattering off impurities fully *ab-initio* [4] into the scattering matrix $M(\vec{k}, \vec{k} + \vec{q})$ in equation (1) with which we calculate the SSP. Thus we study the JDOS, the SSP and the scattering properties of different impurities at the surface of the strong topological insulator Bi₂Te₃, including all effects such as the hexagonal warping of the Fermi surface and correct self-consistent charge and spin screening of the impurity. In our calculations we employ the full potential relativistic Korringa-Kohn-Rostocker Green function method within density functional theory for the electronic structure and scattering properties at defects [4,5].

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Topological Crystalline Insulator and Quantum Anomalous Hall States in IV-VI based Monolayers and their Quantum Wells

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The topological crystalline insulator (TCI) is a new class of quantum states in both two and three dimensions which exhibits metallic boundary states protected by crystal mirror symmetry, in contrast to Z_2 topological insulators (TIs) that rely on time-reversal symmetry [1-2]. TCIs bear great potential for the investigation of exotic phenomena, such as strain-induced superconductivity or the quantum anomalous Hall (QAH) effect with large Chern numbers. While theoretical and experimental progress in the field of 3D TCIs was rapid, the 2D TCI was predicted to exist in freestanding films only recently [2]. However, the 2D TCI phase disappears when the mirror symmetry is broken upon placing on a substrate, which greatly obstructs its further experimental investigation and device application.

We theoretically predict that both the SnTe and the PbTe (001) monolayers are 2D TCIs with mirror Chern number $n_M = -2$, despite the fact that their parent bulk compounds display different topological properties [3]. When exposed to an exchange field, which mimics the effect of magnetic adatoms or substrates, we find that an in-plane exchange field destroys the TCI phase, while it survives for an out of plane magnetization. At appropriate strength of the exchange field, as the Chern number and edge state analysis show, the QAH state with Chern number $C = +2$ is obtained, which is very robust to mirror symmetry breaking and/or magnetization fluctuations. Remarkably, we find that the mirror symmetry and TCI phase survive when the monolayers are sandwiched between slabs of NaCl of various thickness. The energy gap of 0.47 eV for PbTe is by far larger than those of known 2D and 3D TCIs, which is desirable for potential applications. Our findings not only reveal a new formation mechanism for large-gap 2D TCIs, but may also pave the way for the experimental realization of the QAH effect in these systems.

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Probing the electronic and structural properties of the first weak 3D topological insulator $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ by scanning tunnelling microscopy

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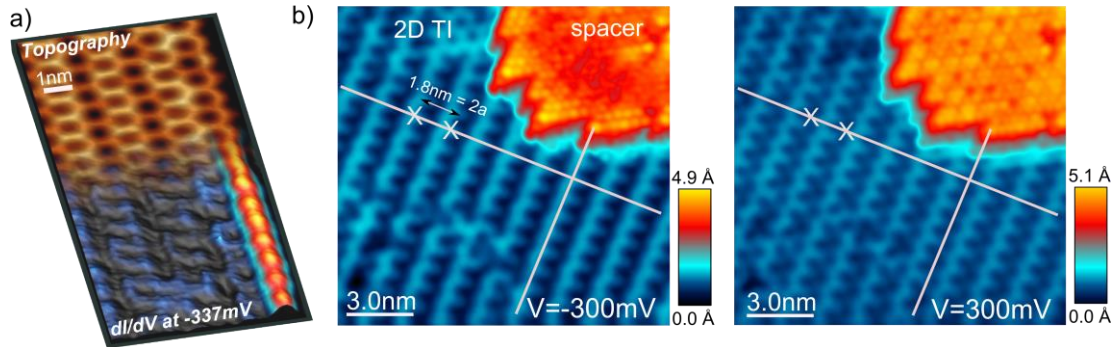
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In this study, we present scanning tunnelling microscopy (STM) measurements at 6 K characterizing the electronic and structural properties of the first weak topological insulator $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ [1-2] on the atomic scale. In [001]-direction, the material is built from stacks of intermetallic planes with non-trivial 2D topology and insulating spacer layers in between. Thus, the surfaces of the 2D topological insulator (TI) layer, which are the natural cleaving planes of the material, exhibit a non-trivial band gap, however, with topologically protected states at each step edge [2]. We checked that the edge state covers the whole non-trivial band gap as well as its spatial continuity along all investigated step edges as required from topology. Even in the presence of strong disorder, the edge state is not interrupted. Further, the width of the edge state is found to exhibit a FWHM of 0.8 nm, showing that it is confined to a single unit cell only (width: 0.92 nm [1]). In addition, a bias-dependent surface modulation of the 2D TI layer as well as a deviation from a perfect honeycomb appearance induced by the different stacking between the 2D TI layer and the underlying zigzag chain structure of the spacer layer was found in excellent agreement with DFT. The absence of the topological edge states in the structural closely related material $\text{Bi}_{13}\text{Pt}_3\text{I}_7$, where stacks are built from pairs of 2D TIs, is in accordance with our results from DFT and general theoretical considerations, and corroborates the topological nature of $\text{Bi}_{14}\text{Rh}_3\text{I}_9$'s edge states.



a) STM topography image of the 2D TI layer (honeycomb lattice) with overlaid dI/dV data ($V_{\text{stab}} = -337$ mV) at the bottom part of the image. Sub-nm wide topological edge state (orange stripe) is present at the step edge of the 2D TI layer. b) STM topography image of the 2D TI and spacer layer recorded at opposite bias voltages (as marked). Bias-dependent surface modulations are visible for both layers as well as a deviation from the perfect honeycomb lattice for the 2D TI layer.

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Experimental Discovery of the Weyl semimetal state in TaAs

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Three types of fermions play a fundamental role in our understanding of nature: Dirac, Majorana, and Weyl. While Dirac fermions have been known for decades, the latter two have not been observed as any fundamental particle in high energy physics and have emerged as a much-sought-out treasure in condensed matter physics. A Weyl semimetal is a novel crystal whose low-energy electronic excitations behave as Weyl fermions. It has received worldwide interest and is believed to open the next era of condensed matter physics after graphene and three-dimensional topological insulators. Here, we present the first experimental discovery of the Weyl semimetal state in an inversion symmetry breaking single crystalline solid, TaAs. Utilizing the combination of soft X-ray and ultraviolet photoemission spectroscopy, we experimentally observe both the Weyl cones in the bulk and the Fermi arcs on the surface of this system. Our ARPES data, in agreement with our theoretical band structure calculations, provide conclusive evidence for the Weyl semimetal state in TaAs and reveal the first complete topological information, both on the surface and in the bulk, of a Weyl semimetal in experiment. Our discovery of the first Weyl semimetal in nature not only paves the way for the many fascinating topological quantum phenomena predicted in Weyl semimetals, but also establishes a new cornerstone in the correspondence between high-energy and condensed matter physics.

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Fabrication and characterization of GaSb/InAs double quantum wells for tunable topological insulator devices

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InAs/GaSb compound quantum wells (CQW) sandwiched between two AlSb barrier layers are proposed by Liu et al. [1] to show a topological phase similar to the one realized in HgTe/CdTe [2]. While in the HgTe/CdTe system the transition from the normal to the topological insulator state can only be tuned by thickness variation, for InAs/GaSb CQWs this is thought to be tunable. Our structures are fabricated by molecular beam epitaxy on both, GaAs substrate combined with buffer structures and GaSb substrate. For the identification of a quantum spin hall state in InAs/GaSb system and the realization of a quantum spin Hall field effect transistor growth, lithography and passivation obstacles have to be overcome. Transport data and reversible switching majority carriers from electrons to holes by optical doping will be shown.

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A combined XMCD, ARPES and STM study of 3d adatoms on the topological insulator Bi₂Te₃

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Topological surface states are protected against direct backscattering due to time-reversal symmetry. Recent results showed that interaction with out-of plane orientated Mn-adatoms in the dilute coverage regime can break symmetry on the topological insulator Bi₂Te₃ [1]. In order to investigate the electronic and magnetic structure of other 3d adatoms adsorbed on bare Bi₂Te₃ we performed x-ray absorption spectroscopy, x-ray magnetic dichroism (XMCD) and angle-resolved photoemission spectroscopy (ARPES). In addition we observed with scanning tunneling microscopy and spectroscopy different adsorption sites for the same single adatoms which is in a good agreement with DFT calculations.

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SPP 1666

Topological Insulators

Materials - Fundamental Properties - Devices

Modification of Atomic, Electronic And Spin Structure of Pb-based Quaternary Topological Insulator With Various Stoichiometry

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Topological insulators (TIs) have attracted a lot of interest in recent years as being a promising material for spintronics application. Due to the strong spin-orbit induced inversion of the band spectra TIs possess unique Dirac-cone like topological surface states (TSSs). These TSSs having a helical spin structure are protected from backscattering providing an opportunity of non-dissipative spin currents along the TI's surface [1].

Up to date electronic and spin structures of wide class of TIs are well studied, however searching for new topological compounds with demanded features of electronic structure (Fermi level as well as Dirac point positions relative to the bulk bands, size of the band gap) is still an ongoing problem now. It was shown that while variation of the third component concentration in Bi-Te-Se series one can slightly change the electronic structure [2]. Whereas in Pb- or Sb-based quaternary TIs the significant modifications are observed [3].

In the present work we report on experimental spin-ARPES study of electronic and spin structure of Pb-Bi-Te-Se series with various stoichiometry and atomic structure together with the theoretical calculations. Studied $\text{PbBi}_2\text{Te}_2\text{Se}_2$ consisting of septuple layers (7L) is predicted to have a wide insulating gap originating from bulk states which is useful for high temperature spintronics and is featured with the complicated spin structure. While $\text{PbBi}_4\text{Te}_5\text{Se}_2$ as well as $\text{PbBi}_4\text{Te}_4\text{Se}_3$ TIs consist of two alternating 7L and 5L blocks weakly bonded to each other by van der Waals interaction and may have two possible surface terminations after cleavage. This fact was shown to have an intriguing appearance in the electronic structure. Namely, the Dirac cone TSS shifts into the underlying 7L out from the top, making it more protected from surface perturbation, and the two Dirac cones become distinguished in ARPES spectra [4,5]. In current work we discuss localization of the Dirac cone TSSs, probed experimentally by using different photon energies and thereby varying the probing depth.

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Nanoconstrictions in Quantum Spin Hall Effect Materials

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Although quantum spin Hall effect is a phenomenon which shows a great promise for quantum spintronics, the accuracy of experimentally observed conductance quantization is not fully satisfactory. Therefore, it is interesting to investigate the reasons for discrepancies between theory and experiment through studying the properties of the edge states, depending on the structure design and disorder. Motivated by experimental studies of quantum point contacts, which follow previous studies [1], we perform transport simulations of quantum spin Hall effect materials by using scattering matrix formalism. We study three different classes of shapes of the point contacts and various sizes of them in each of the classes. Parameters of the constriction for which the topological protection ceases to operate are determined. Those parameters show a strong dependence on the position of the Fermi level inside the bulk band gap. A comparison is made between the impact of the correlated and uncorrelated disorder on the conductance of the samples. We establish the dependence of the decay length of the edge states on the disorder strength and Fermi energy. We map the simulation results onto the experimental results and tell to what extent alloy fluctuations in the barrier and residual impurities in the well may account for breaking of the topological protection, if a weak time-symmetry breaking mechanism is allowed. We also investigate interferometers formed from multiple quantum point contacts arranged in series. We show how by adjusting the magnetic field flux through the samples one can control the probability of transmission through the interferometer and how its properties change depending on the geometry of the contacts and the disorder in the sample.

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Ultrafast Electron Dynamics of the Topological Insulator Sb_2Te_3 Studied with Tunable Pump Photon Energies

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The understanding of the optical excitation of topological surface states (TSSs) and their electron dynamics is a key for an optical control of spin-transport and spin-orientation. Time- and angle-resolved two-photon photoemission (2PPE) is a particularly well suited technique for this purpose, because it directly visualizes the population dynamics of optically excited states in momentum space. Previous studies of topological insulators using 2PPE, however, typically suffer from an excitation of the TSS which is dominated by an indirect filling from higher lying states. This indirect filling prohibits optical control and makes it difficult to extract the true electron dynamics in the TSS.

Here, we report on time- and angle-resolved 2PPE investigations of p-doped Sb_2Te_3 where we try to overcome the drawbacks of an indirect filling of the TSS. Based on previous work [1] on the ultrafast electron dynamics in the TSS using visible pump pulses (2.58 eV) and ultraviolet probe pulses (5.15 eV), we have extended our laser setup for the use of mid- to near-infrared pump pulses (0.2 eV to 1.0 eV). We will show that the reduction of the pump photon energies makes it possible to suppress the indirect filling. Independent of the pump photon energy, the overall dynamics of the electrons in the TSS below the conduction band minimum show an decay on a picosecond timescale.

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4π contribution to the Josephson supercurrent in a HgTe based topological Josephson junction

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3D topological insulators are a new class of material in which electronic transport is governed by topological surface states with helical spin polarization and a Dirac like band dispersion. Besides the new fundamental physics inherent to such surface states, the coupling to conventional s-wave superconductors may lead to the emergence of new exotic phenomena such as induced p-wave with a unique gapless zero-energy Andreev bound state [1]. This Andreev bound state is topologically protected against backscattering and thus gives rise to a 4π -periodic Josephson current.

In this work we use strained HgTe as a three dimensional topological insulator which exhibits low carrier densities and high mobilities [2]. We fabricate lateral Josephson junctions based on a HgTe weak link and deposit niobium contacts. The behaviour of the junctions show large and reproducible supercurrents. Additionally the observation of an excess current highlights the high quality of the devices. By applying microwaves to the junction, we study the A.C. Josephson effect and the formation of the so-called Shapiro steps. We observe a doubled first step in the A.C. Josephson response and explain this anomalous behaviour by a presence of a 4π -periodic supercurrent. Furthermore we show that the contribution is compatible with the presence of a gapless zero-energy bound state.

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Pressure Induced Topological And Crystal Phase Transitions In BiTeX (X=I, Br, Cl)

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Fabrication of the advanced materials and devices for the high-tech industry use is widely based on the nanostructured systems which exhibit unique properties due to their small size and complex structure of the material. The theoretical studies related to the topological insulators and bismuth tellurohalides BiTeX (X=I, Br, Cl) - fundamentally new materials that simultaneously combine the properties of both semiconductor (in the bulk) and metal (on the surface). They can be used for creation a topological quantum computer and, in combination with ferromagnets, for the development of a new type of magnetic memory devices, based on the effect of the spin rotation, as well as, in combination with superconductors, for creation of a new type of superconducting materials.

Evolution of electronical structure of BiTeX (X=I, Br, Cl) under the external pressure is actual task in the spintronics due to possibility of changing spin splitting parameters in these compounds and in such a way of controlling their transport properties. In the investigation we interested by the gap width, Rashba spin-splitting parameters of gap edge states as functions of the pressure. On the basis of enthalpies comparison at possible structures of the reviewed compounds, the crystal phase transitions was investigated. The topological phase is also traced with increasing of the pressure. For each compound the conclusion about the possibility of topological phase transitions in the investigated compounds was done.

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Tuning the Dirac Point Position in Bi_2Te_3

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In the last few years, there is a booming in the field of topological insulators representing a new state of quantum matter and combining the properties of the semiconductor in the bulk and the metal on the surface (5-10 atomic layers). Topological insulators (TIs) possess an enormous potential for applications in spintronics and quantum computing. To date, the number of prototype devices exploiting unique properties of TIs have already been proposed. These devices are expected to operate faster, consume less power and have much smaller size than the nowadays devices. Currently, the challenge in this field is the design of new topological insulators with desired characteristics and the search of the ways to control their electronic properties in order to realize technologically important effects at room and higher temperatures.

Using ab initio calculations, we show a promising way to control the Dirac point in Bi_2Te_3 within the bulk band gap. The ultrathin film deposition on Bi_2Te_3 leads to shifting of the Dirac point up to valence band maxima which allows eliminate scattering between the upper cone and the bulk continuum states inherent to Bi_2Te_3 . Our study suggests a new path to actively modify the topological surface state in TI.

Strongly anisotropic spin-orbit splitting in a two-dimensional electron gas

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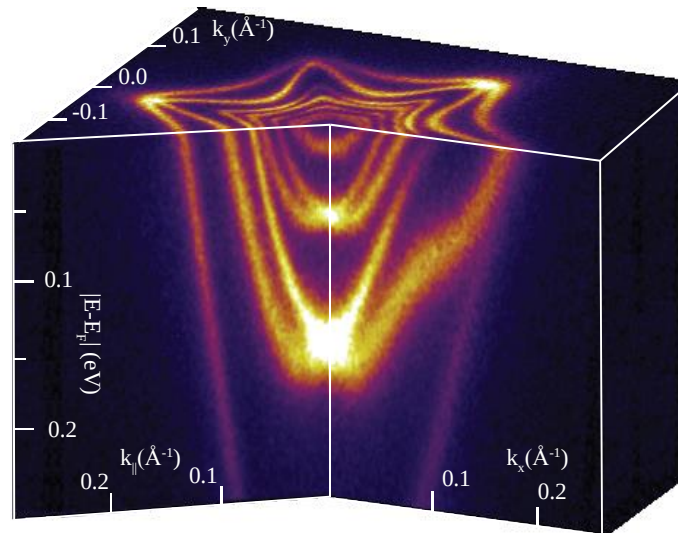
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Near-surface two-dimensional electron gases on the topological insulator Bi₂Te₂Se are induced by electron doping and studied by angle-resolved photoemission spectroscopy. A pronounced spin-orbit splitting is observed for these states. The k-dependent splitting is strongly anisotropic to a degree where a large splitting ($\approx 0.06 \text{ \AA}^{-1}$) can be found in the $\bar{\Gamma} \bar{M}$ direction while the states are hardly split along $\bar{\Gamma} \bar{K}$. The direction of the anisotropy is found to be qualitatively inconsistent with results expected for a third-order anisotropic Rashba Hamiltonian. However, a k·p model that includes the possibility of band structure anisotropy as well as both isotropic and anisotropic third order Rashba splitting can explain the results. The isotropic third order contribution to the Rashba Hamiltonian is found to be negative, reducing the energy splitting at high k. The interplay of band structure, higher order Rashba effect and tunable doping offers the opportunity to engineer not only the size of the spin-orbit splitting but also its direction.



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Search for new topological insulators among halogen-containing Tl_5Te_3 structural derivatives

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The Tl_5Te_3 -type materials have been recently recognized as promising candidates combining topological surface states and bulk superconductivity [1]. Sn-doping was predicted to induce a topological phase transition in $\text{Tl}_4\text{Tl}_{1-x}\text{Sn}_x\text{Te}_3$; however, both Tl_5Te_3 and Tl_4SnTe_3 are shown to exhibit metallic conductivity [1, 2]. Our research aims at the search for new non-metallic derivatives of the Tl_5Te_3 type. We show that semiconductors are accessible by halogen $X = \text{Cl}, \text{Br}, \text{I}$ substitution in the Te sublattice of Tl_5Te_3 , thus yielding $\text{Tl}_5\text{Te}_2\text{X}$ compounds. Their single crystals are obtained by slow cooling of the melts.

The band structure analysis (DFT, GGA, QUANTUM-ESPRESSO package [3]) shows that without spin-orbit coupling $\text{Tl}_5\text{Te}_2\text{Br}$ is a semimetal with the conduction and valence bands crossing along a line around the Γ point. Spin-orbit coupling lifts the degeneracy along this line to form a semiconductor with an inverted band at Γ and a band gap of ~ 0.057 eV. However, the computed $\mathbb{Z}_2$ topological indices are (0,000); hence $\text{Tl}_5\text{Te}_2\text{Br}$ is topologically trivial. The analysis of the change of parity of the occupied bands at the TRIM points shows that the two inverted bands possess the same parity at Γ and that their inversion does not lead a $\mathbb{Z}_2$ topological phase.

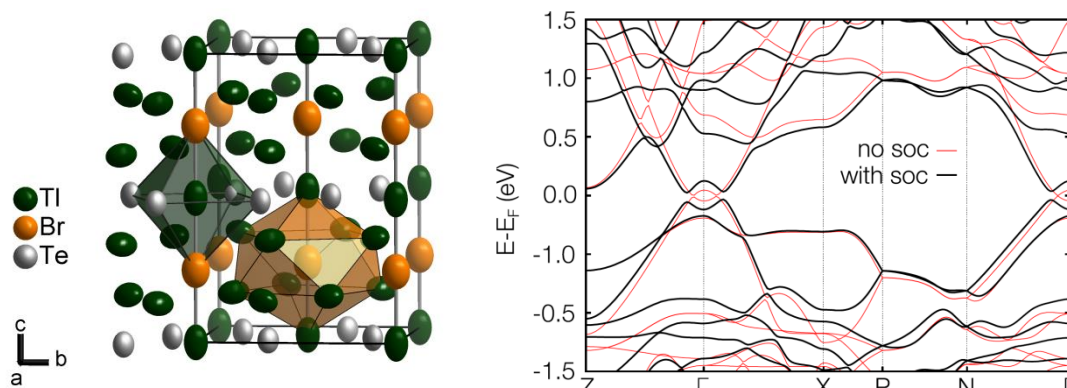


Fig. 1. Crystal structure of $\text{Tl}_5\text{Te}_2\text{Br}$ (left) and its electronic band structure (right)

This work is supported by the Swiss NSF, the ERC “TopoMat” and the DFG SPP 1666.

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Ferromagnetic iron as a topological metal

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Topological metals are a recently-proposed phase characterized by the presence of disconnected Fermi surface (FS) sheets with nonzero Chern indices^[1]. This requires breaking the effective symmetry PT obtained by combining spatial inversion (P) with time-reversal (T). Under these conditions most accidental degeneracies are lifted, except for isolated band touchings and a few line nodes on mirror planes. The isolated band-touching points (Weyl nodes) can not be easily removed, and act as monopoles of Berry curvature, which in turn gives rise to the intrinsic anomalous Hall conductivity (AHC). The Chern number of each individual FS sheet is given by the net enclosed topological charge. Here we show that when the effect of spin-orbit coupling is taken into account, ferromagnetic bcc iron is a P -invariant, T -broken metal, and analyze the implications for the AHC. First we carry out a systematic search for band touchings in the bandstructure, using first-principles calculations. We find numerous degeneracies, mostly Weyl points (linear crossings) carrying charge ± 1 , but also several double-Weyl nodes (quadratic band touchings) with charge ± 2 . Nevertheless, most FS sheets are topologically trivial, with zero Chern index. The reason is that they surround P -invariant points in the BZ, so that the enclosed Weyl nodes come in pairs of equal and opposite charge. The exceptions are two small electron pockets on the Δ line parallel to the magnetization. Each of them encloses a single Weyl node, leading to Chern indices of ± 1 . The contribution of these two pockets to the AHC is given, modulo a G vector, by their reciprocal-space separation, as in a magnetic Weyl semimetal. We mimic the effect of heterovalent alloying by shifting the Fermi level, and find that under a small upwards shift the Chern numbers on the two pockets flip their signs. This happens via a concerted event where both pockets simultaneously touch a large Fermi sheet in the band below, exchanging respectively $+2$ and -2 amounts of Chern number with it.

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Magneto-optical and magneto-transport signatures of giant Rashba splitting in BiTeBr and BiTeCl

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Layered bismuth chalcogenides BiTeX (where X=I, Br or Cl) host giant Rashba spin splitting, which makes these materials interesting for spin manipulation.

We present a comparative study of the optical properties - reflectance, transmission and optical conductivity - and Raman spectra of BiTeBr and BiTeCl at 300K and 5 K. Despite different space groups, the optical properties of the two compounds are very similar. Both materials are doped semiconductors, with the absorption edge above the optical gap which is lower in BiTeBr (0.62 eV) than in BiTeCl (0.77 eV). The same Rashba splitting is observed in the two materials. A non-Drude free carrier contribution in the optical conductivity as well as three Raman and two infrared phonon modes are observed in each compound. There is a dramatic difference in the highest infrared phonon intensity for the two compounds, and a difference in the doping levels. Aspects of the strong electron-phonon interaction are identified. Several interband transitions are assigned, among them the low-lying absorption “beta” which has the same value 0.25 eV in both compounds and is caused by the Rashba spin splitting of the conduction band. An additional weak transition is found in BiTeCl, caused by the lower crystal symmetry.

We performed a detailed study of reflectivity and Kerr effect on BiTeBr and BiTeCl up to a field of 7 T and in a wide energy range from 2 meV to 0.5 eV. We find a large Kerr effect in BiTeBr in the far infrared (with Kerr rotation up to 0.15 rad) and a smaller but qualitatively similar response in BiTeCl.

In a similar vein, magneto-transport study was performed on these samples at temperatures down to 1.5 K and p to 7.5 T.

The analysis of the optical Kerr data and the magnetic transport data is done in terms of the Rashba split bands.

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Systematics Of Hybrid Organic-Topological Insulator Heterostructures

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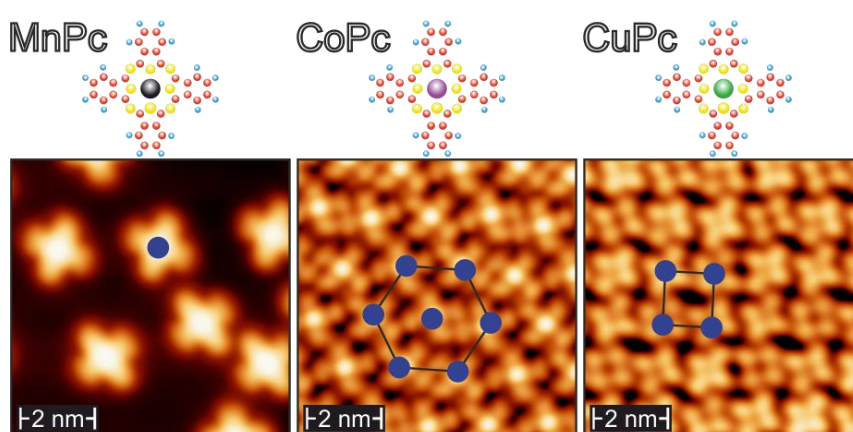
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Topological states promise to be an ideal platform for spintronic applications. These intimately depend on the ability to couple their helical spin states to well-defined perturbations. However, up to now, TI-based heterostructures always resulted in very disordered interfaces, characterized by strong mesoscopic fluctuations of the chemical potential that make the spin-momentum locking ill-defined over length scales of few nanometers or even completely destroy topological states. These limitations call for the ability to control topological interfaces with atomic precision [1, 2].

Here, we report a combined low-temperature scanning tunneling microscopy and spectroscopy study of the prototypical interface between transition metal phthalocyanine (TMPC) molecules coupled to Bi₂Te₃. Our findings show that appropriate chemical modifications, i.e. varying the TM-atom, it is possible to tune the balance of molecule-substrate and molecule-molecule interactions. This may trigger self-assembly processes which create well-organized molecular superstructure of different symmetries. Our results identify hybrid organic-TI interfaces as ideal heterostructures for tailoring potential landscapes at TI surfaces, with a precision down to the atomic scale [3, 4].



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Spin-resolved ARPES as a probe for the phase of the photoelectron wavefunctions

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Spin- and angle-resolved photoemission spectroscopy (SARPES) is a unique and well established technique which has been intensively used to measure the spin structure in systems with spin polarized initial states such as Rashba systems [1] and topological insulators [2]. However, the spin polarization of the photoelectrons can also originate from the photoemission process, and it can be present even when the initial state is not spin polarized thanks to quantum interference of different wavefunctions [3], thus carrying information about the process itself. In particular, the dynamical spin polarization parameter ξ is related to the phase shift between the interfering wavefunctions [4]. It is noteworthy that a completely different approach to obtain access to the phase shift information became feasible in the recent years: time-resolved ARPES in the attosecond regime [5]. In this method the measured time delay is related to the phase shift via the Eisenbud-Wigner-Smith model [6].

Whereas the formalism regarding the spin polarization of electrons from photoionization of atomic targets is quite well developed since decades [7], a complete model for the case of photoemission from solid state targets is missing. Here the first systematic measurements of the spin polarization from spin degenerate initial states are discussed. We investigated the photoemission from free-electron-like *sp* bulk-derived band of Au(111) and Cu(111). Despite the simplicity of these textbook systems considered as a first step, they show a rich variety of spin effects. A clear spin signal is observed with a not yet fully understood dependence on the various photoemission parameters such as photon energy, kinetic energy, and geometry. Nonetheless, thanks to a simple model extended from the atomic case and still under improvement we are able to extract from these first results a value for the phase shift which directly corresponds to a time delay in the attosecond scale.

It is clear that in addition to a deeper insight into the dynamics of the photoemission process itself, the access to the phase information with SARPES would give a significant contribution to the understandings of more interesting compounds, such as strongly correlated electron systems or novel topological phases. For example, a clear understanding of such bulk spin signals will be essential for SARPES on the bulk states of Weyl semimetals.

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Laser induced DC photocurrents in a Topological Insulator thin film in the transition from p- to n-doping

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Topological Insulators (TI) potentially open up a novel route to influence the transport of charge or spin in a functional thin film in a unique way. The energy momentum landscape of the Dirac cone provides via spin-momentum locking of the current and the spin a control of the directionality of spin and momentum ^{[1][2]}. The underlying transport effects of DC detected polarization dependent photo currents still demands clarification of their contribution. The thermoelectric, photogalvanic and the photon drag effect have to be set in relation with the crystal's or the effect's symmetry ^[3] and the alignment of the exciting field components of the used light ^[4]. In result it is possible to distinguish between them and track the effect of the topological surface states light driven spin-polarized currents.

Therefore we present our results on laser excitation (1.58 eV) in TI thin films, structured to Hall bar devices for DC lock-in measurements with focus on the periodicity in polarization dependence of the lasers light. Our thin film thickness is in the range of some quintuple layers (20 nm tops) of the crystal and the doping type transition from n- to p-type via the composition between antimony (Sb) and bismuth (Bi) with tellurium (Te). Thereby minimizing bulk contributions and controlling the electronic density around the Dirac point. In addition we discuss interpretation for optical transition and transport with focus of the geometry of exciting light and the crystal's symmetry by selectively exciting the spin states with right and left circularly polarized light. The effect of thermo currents arising at the same time are although considered.

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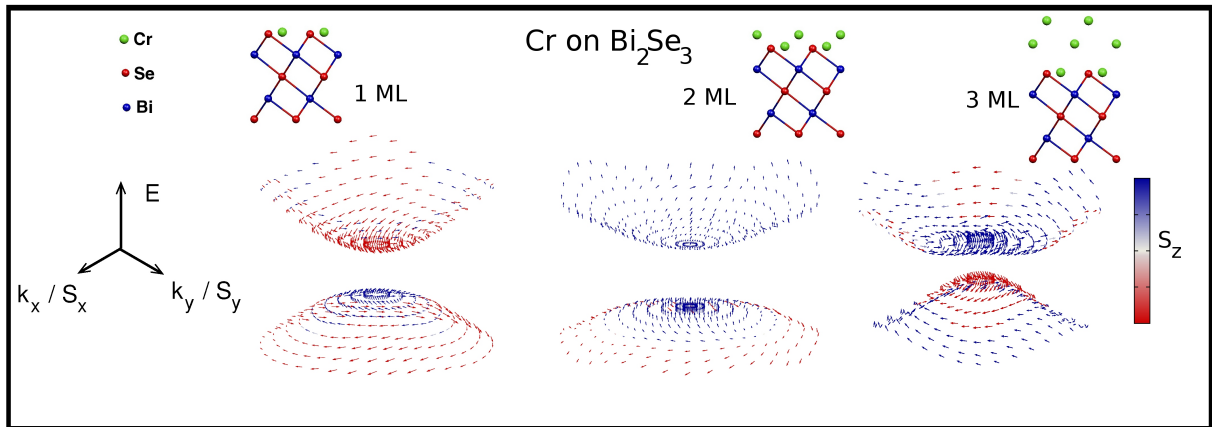
Oscillatory exchange coupling and massive Dirac state spin texture in Cr thin films coupled to Bi₂Se₃ surfaces

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Topological insulators (TIs) are characterized by metallic surfaces with topologically protected helical spin Dirac surface states (SSs). In magnetically doped 3D TIs the interplay of topological protection and broken time reversal symmetry (TRS) leads to exotic magnetoelectric effects [1]. Here, we investigate the effect of Cr ultrathin films adsorbed on the surface of the TI Bi₂Se₃. The Cr film breaks TRS, destroying the topological protection of the SSs and opening a small gap in the energy spectrum. For ultrathin films -1 to 4 monolayers (MLs)- the surface Dirac gap opened by the exchange interaction is of ~100 meV, almost independent of the Cr thickness. However, Cr films also alter the Bi₂Se₃ electronic structure by hybridisation and, depending on the thickness, shift the Fermi energy within the bulk band gap. For 3 MLs E_F is located within the surface Dirac gap. Close to the Γ point, the spin of the massive Dirac quasiparticles lies in the z direction perpendicular to the surface, while the original in-plane spin-helicity of the undoped TI is preserved at high momenta. Furthermore, the sign of S_z for the resulting electron-like (ESS) and hole-like (HSS) surface bands oscillates with the number of Cr atomic layers on the Bi₂Se₃ surface and therefore can be tuned by controlling the deposition process. Several magnetic configurations are found, with S_z of ESS and HSS aligned parallel or antiparallel. The magnetic order of the Cr layers oscillates between ferro- and antiferromagnetic alignment. We discuss the origin of the magnetic order considering both the direct exchange among the Cr atoms, and the massive Dirac SS-mediated RKKY mechanism [2]. Our results indicate that a reversal of the electron spin could be achieved by means of a very small electric field in this kind of structures, paving the way for the development of TI based spintronic devices.



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Ultrathin Tetradymite-like 3D Topological Insulators

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The use of topological insulators (TI) in spintronics opens up new perspectives in development of devices with unique properties and characteristics. It is known that on the surface of a semi-infinite crystal of the TI there exist spin-polarized surface states with a characteristic linear dispersion in the form of the Dirac cone. Such states are topologically protected from backscattering on crystal defects and non-magnetic impurities.

In the currently known TIs the Dirac cone is completely formed on the surface of the 30 – 40 atomic layer film, which corresponds to the thickness of about 50 – 60 Å. Miniaturization of devices requires a search for materials where 3D electronic topological properties could be realized in films with smaller thickness.

In the present work we study by first-principles density-functional methods the electronic structure of the tetradymite-like TIs and demonstrate that in this system three-dimensional topological properties are realized already in the ultrathin films of thickness of 25 – 35 Å. It was found that these compounds have a wide band gap of about 300 meV and the Dirac cone surface states are characterized by a high spin polarization.

Observation of gapped surface states in the topological regime of the quantum-phase transition in Bi-doped Pb-Sn-Se (111) epitaxial films

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Using angle-resolved photoemission, we investigate (111) oriented epitaxial films of pristine and Bi-doped $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ grown by molecular beam epitaxy. We monitor the topological to trivial insulator quantum-phase transition [1] by probing the electronic structure as a function of Sn concentration at temperatures down to 30 K. Differently from the case of the (001) surface [2], we observe two types of Dirac cones centered at $\bar{\Gamma}$ and $\bar{M}$ originating from the band inversion at the L -point of the bulk Brillouin zone. By comparing the band structure of samples with fixed Sn concentration and different Bi doping, we demonstrate the existence of gapped surface states within the topological regime of the quantum-phase transition at low temperatures. We discuss the origin of the gapped surface states in connection to Bi doping, which is not expected due to protection by time-reversal symmetry [3].

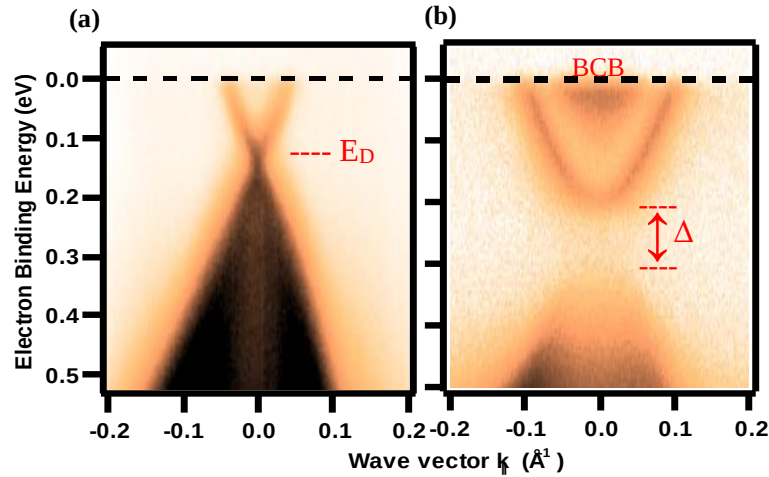


Fig. 1: ARPES spectra of (111) $\text{Pb}_{0.72}\text{Sn}_{0.28}\text{Se}$ epilayers (a) without Bi doping where the Dirac node (E_D) is intact, and (b) after 2.2% Bi doping revealing the opening of a large gap (Δ) in the original Dirac node. The bulk-conduction band (BCB) is clearly observed due to the additional doping. Measurements are taken at 30K and 18 eV photon energy.

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Terahertz Spectroscopy of 2D and 3D Topological Phase Transition

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Recently, a type of topological invariance was predicted in materials with band inversion due to strong spin-orbit coupling. In this case, one speaks of topological insulators.¹ This kind of topologically protected surface state was first demonstrated to exist in two-dimensional HgTe/CdTe quantum wells (QWs).^{2,3} In this work, we report on a Terahertz magneto-photoconductivity study of inverted band structure HgTe-based Field Effect Transistor (FET) : i) We observe a resonance that could be attributed to topological phase transition related to anticrossing of the zero-mode Landau levels at a critical value of the magnetic field⁴. ii) We also observe unknown resonances in the direct band structure regime which are shifting to higher magnetic field values with increasing gate voltage. These resonances cannot

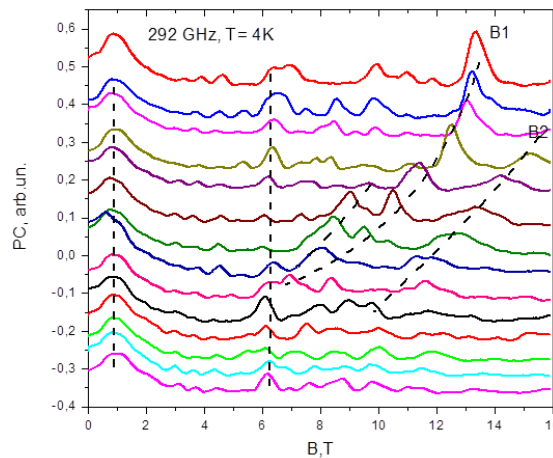


Fig. 1 Photoconductivity spectra as a function of magnetic field for different values of gate bias, at 292 GHz and 4K.

be attributed to magnetoplasmons and may be linked with impurity resonant transitions. iii) We finally observe the cyclotron resonance line giving electron effective mass $m^* = 0.03 m_0$.

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***Ab initio* study of adsorption and diffusion of the I-, IIA- and IIIA- group adatoms on the surface of topological insulator Bi₂Se₃**

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Adsorption of the alkali metal atoms on the surface of topological insulator (TI) Bi₂Se₃ was recently found to induce the appearance of a two-dimensional electron gas states with a strong Rashba splitting [1-2] that could be used to realize spin field effect transistors.

Here we present a systematic *ab initio* study of adsorption and diffusion of alkali, alkaline-earth and boron group atoms on the Bi₂Se₃ surface. The calculations are performed using the projector augmented-wave method in the VASP implementation. The adsorption energy and geometry as well as the charge transfer for each adatom/Bi₂Se₃ system are calculated. The diffusion activation energies of adatoms on the surface have been calculated using the nudged-elastic-band method. Based on the activation energies obtained, we estimate the diffusion length as a function of temperature for all the adsorbates under consideration making use the formalism proposed in [3]. The results obtained are discussed in the context of available experiments.

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High temperature Quantum Hall Effect in HgTe/HgCdTe quantum wells with a bulk band gap

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Two-dimensional (2D) topological insulators (TIs) are a new class of materials that are insulating in the bulk while conducting at the edge. This peculiar system can be achieved in HgTe/CdTe quantum wells (QWs) which possess an inverted band order when the QW thickness d exceeds a critical thickness d_c . In this inverted regime, the system is characterized by a finite bulk band gap with conducting helical edge states [1].

In this work we present magneto-transport data of inverted and non-inverted HgTe/HgCdTe up to 30 T in order to investigate the high temperature limit of the Quantum Hall Effect (QHE). Large energy gaps in the Landau level spectrum occur because of the Dirac like dispersion of charge carriers (Fig. 1a)). These calculations are based on the 8×8 $\mathbf{k} \cdot \mathbf{p}$ model [2]. The energy gap at filling factor $\nu=1$ even exceeds the thermal energy at room temperature for $B > 20$ T, showing that this system is suitable to investigate the QHE at high temperatures.

In measurements of the longitudinal resistance and the Hall conductivity σ_{xy} we observe pronounced Shubnikov-de Haas oscillations up to 63 K and a quantized Hall conductivity up to 46 K at $\nu=1$ (Fig. 1 b) and c)). Notably, the ratios between the thermal energy and extracted energy gap at filling factors 1 and 2 are of the same order of magnitude as found in the room temperature experiment in graphene on SiO₂ [2].

Based on calculations and magneto-transport experiments, we intend to elucidate the importance of localized states for the high temperature limit of the QHE.

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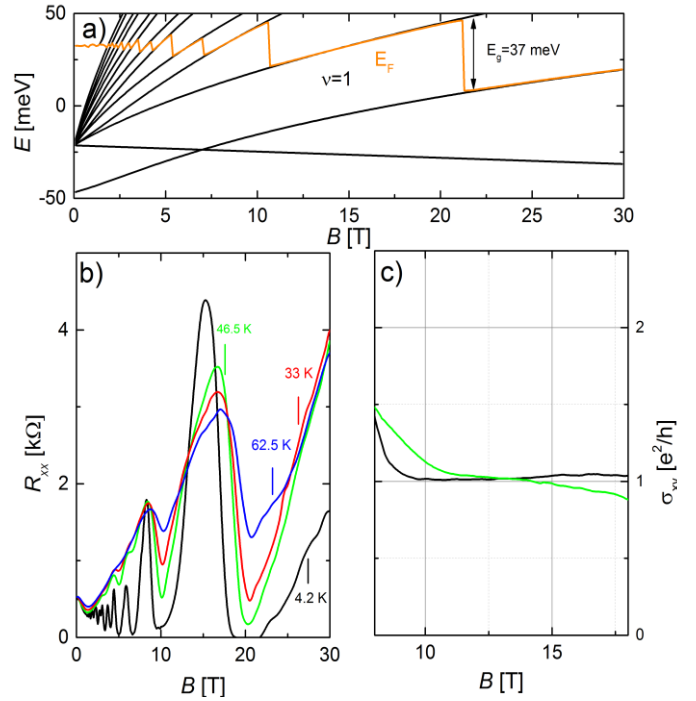


Fig.1 a) Calculated Landau level spectrum for a 11 nm thick QW. Magneto-transport measurements of the b) longitudinal resistance R_{xx} and c) Hall conductivity σ_{xy}

Tuning the first weak 3D-TI $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ for transport measurements

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The layered compound $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ is the first experimentally realised weak three-dimensional topological insulator (TI) [1]. It consists of intermetallic layers with edge-sharing rhodium-centred bismuth cubes that are separated by ionic spacer layers. The hexagonal intermetallic layer resembles the structure of graphene and is predicted to exhibit the quantum spin hall (QSH) effect, which makes it “graphene with strong spin orbit coupling”.

The calculated band structure was confirmed via angle-resolved photoelectron spectroscopy (ARPES) [1]. Lately, scanning tunnelling microscopy (STM) revealed the predicted [2] electronic edge states on the edges of the terraces on the “dark surface”, which is identical with the cleaving surface [3]. These states have been shown to be topologically non-trivial, as they are continuous in space and energy.

So far, conductivity measurements have shown metallic transport behaviour, despite the insulating state predicted for $\text{Bi}_{14}\text{Rh}_3\text{I}_9$ by DFT-calculations. This result concerts with ARPES and STM, as there the Fermi level was found to lie within the conduction band.

Judging from the salt-like layered structure, we anticipate that the termination of the cleaving (“dark”) surface should have a strong influence on the Fermi level. To address this issue, we computed the electronic structure of a finite slab that comprises two intermetallic layers and two spacers. This calculation shows that the terminating layers exhibit significant band bending, which could account for a Fermi level shift. While the spacer should be able to mend this problem via iodine non-stoichiometry, the intermetallic layer cannot flexibly vary its charge. This hypothesis accords well with the observed surface structure in STM and with the spectroscopy data. This situation was also modelled in further DFT-calculations, supporting our idea.

Based on these findings, we propose the following solutions for transport measurements: (1) oxidation of the intermetallic layer with iodine after contacting and (2) back-gating of a very thin flake of $\text{Bi}_{14}\text{Rh}_3\text{I}_9$. If our hypothesis of bent bands in the surface QSH layer is correct, both experiments should have impact on the transport properties. At best, the Fermi level would shift into the insulating gap, rendering the sample semiconducting.

We acknowledge support by the German science foundation (DFG). We are indebted to ZIH TU Dresden for provided computational facilities.

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High Frequency Capacitance Measurements In Three-Dimensional Topological Insulators

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The advent of Dirac-matter, most notably topological insulators, is expected to revolutionize the designs and concepts of device technology. More specifically, topological surface states having a mobility and a robust protection against backscattering, are highly suitable for implementation in high-frequency transistors. We thus investigate electron transport in top-gate three-dimensional topological insulator (TI) devices in the high-frequency regime up to 40GHz. Inspired by work on graphene [1] metal-oxide-TI devices are patterned on MBE-grown Bi₂Se₃ film and as well on exfoliated Bi₂Se₃ and Bi₂Te₃. Such gate-drain devices simultaneously allow the application of a gate voltage and measurement of the quantum capacitance C_q in the RF regime. Knowledge of the full (complex) admittance spectrum permits the extraction of the capacitance, the resistance and the contact resistance formed by the TI-metal contact in a “two-point” design. C_q is directly related to the electron compressibility (density of states) of the sample. Measuring the conductivity σ and the density of states simultaneously, by virtue of the Einstein relation $\sigma = C_q D$, we can extract the (electron) diffusion constant D , related to the scattering time in our samples. We extract a quantum capacitance of 20 fF/ μm^2 , what corresponds to approximately the double of graphene’s C_q at the Dirac point and a diffusion constant of $D \approx 430 \text{ cm}^2/\text{s}$. Our measurement of the diffusion constant does not rely on any assumptions concerning the precise band-structure of the material which is often ambiguous due to band-bending and impurity bands. Furthermore, the mobility of parasitic bulk / impurity bands is expected to be smaller than that of a topological surface state. Such a difference in mobility is expected to be eventually noticeable in the high frequency limit (due to a “freezing out” of the bulk carrier motion). Furthermore, if a gate permits to tune the Fermi level, the energy dependence of the diffusion constant might allow to distinguish between different scattering mechanisms.

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ARPES Characterization of the Surface Modified Kondo Insulator SmB₆

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40 years after its first investigation SmB₆ has returned to the focus of interest, because it is predicted to be the first topological Kondo insulator [1] and hereby the first correlated topological insulator at all.

The numerous experimental studies published over the past years have neither been able to confirm nor disprove this prediction. Recently, an unexpected explanation of SmB₆'s unusual conductivity behavior has been found: Instead of topological surface states, two trivial states - a surface component of the f-d-hybridization and a surface dependent Rashba split state - have been identified to be responsible for the remaining conductivity at low temperatures [2]. Since an understanding of the discrepancy between theory and experiment, the surface superstructure, the robustness of the surface conductivity and particular the vanishing surface conductivity of samples with magnetic Gd impurities [3] has not been found yet, further studies concerning the surface composition and the band structure and are indispensable.

With ARPES experiments at well-defined boron or samarium terminated samples and Sm- and Gd-evaporation experiments we contribute to the understanding of the origin and assignment of the electronic structure and the surface composition.

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Searching for Majorana Modes in Mo-S₂-Superconductor Heterostructures

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Majorana quasiparticles have been proposed as ideal candidates for topological quantum computation since they obey non-Abelian statistics and certain of their properties are protected against local perturbations [1,2]. Recent theoretical works [3,4] predict the appearance of Majorana bound states at the edges of single-layer transition-metal dichalcogenides (TMDC) MX_2 ($M = \text{Mo, W}$; $X = \text{S, Se}$) when placed on the surface of a conventional superconducting substrate.

Our aim is to find experimental evidence of the existence of Majorana modes in such TMDC-superconductor heterostructures. We have built hybrid devices formed by a MoS_2 monolayer deposited on a NbSe_2 substrate, where MoS_2 is a semiconductor with strong spin-orbit coupling and NbSe_2 is an s-wave superconductor. Due to proximity effect, one-dimensional *topological superconductivity* is expected to emerge at the edges of the MoS_2 layer, providing the necessary conditions for the observation of Majorana bound states.

Both STM and transport measurements will be performed in order to characterize the proximity-effect-induced superconductivity on the MoS_2 layer. If topological superconductivity is induced at the edges, we expect to observe zero energy anomalies in both transport and STM measurements, which have been regarded as a signature of Majorana modes in other condensed matter systems [4-5].

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Quasiparticle spectrum and bulk plasmons dispersion in the topological insulator Sb_2Te_3

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We present first-principles one-shot *GW* results on the dispersion of the bulk band-gap edges in the three-dimensional topological insulator Sb_2Te_3 . We show that, independently of the reference density-functional-theory band structure (LDA or GGA) and the crystal-lattice parameters used, the *GW* corrections enlarge the fundamental band gap, bringing its value in close agreement with experiment. These corrections also cause the displacement of the valence-band maximum (VBM) to the Γ point, ensuring that the surface-state Dirac point lies above the VBM in agreement with experimental observations. This is of great importance, since the relative energetic position of the Dirac point and the VBM is a decisive factor in the question whether the topological transport regime can be realized in a given TI.

We extend our study to the analysis of the electron-energy-loss spectrum (EELS) of bulk Sb_2Te_3 . The EELS calculated within the random-phase approximation are characterized by low- and high-energy bulk plasmon peaks, and additional two peaks at higher energies that derive from transitions from semicore states. We showed that the EELS up to ~ 30 eV are largely unaffected by the underlying band structure (LDA, GGA, or *GW*, with or without spin-orbit interaction), or by different sets of lattice parameters and atomic positions. These factors have, however, a moderate effect on the peaks that arise from excitations from the semicore states (above 30 eV). Our calculations also revealed a linear and parabolic dispersion for the low- and high-energy bulk plasmons, respectively. The parameters of these dispersions are very close to those found experimentally for the similar compound Bi_2Se_3 .

Progress on Time-of-Flight Momentum Microscopy Towards μm and meV Photoelectron Spectroscopy

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Angle-resolved photoelectron spectroscopy (ARPES) is the key technique to study the electronic structure in solids and has been used extensively to investigate topological insulators [1]. On the other hand photoelectrons can also be used to access real space information about the surface structure, composition and homogeneity via ToF-PEEM [2]. In a collaboration of U. Mainz and MPI Halle ToF detection was combined with momentum microscopy. In combination with a hemispherical analyzer k-microscopy has previously set a benchmark in k-resolution [3], here we report on the ToF approach. One key feature of the instrument is the ability to choose a microregion on the sample, which can be as small as a few μm , possibly even below 1 μm . Electrons emitted from the desired area of the sample are selected by a field aperture within an intermediate image plane in the microscope column. This approach poses no challenge on fine focusing of the photon beam by zone plates etc.

Recent improvement in energy and momentum resolution ($\Delta E = 20 \text{ meV}$, $\Delta k = 0.01 \text{ \AA}^{-1}$) enabled us to resolve the spin splitting of the unoccupied part of the Shockley surface state in cesiated Au(111) by 2PPE (see Fig 1 (b-d)). Sub-monolayer coverage of Cs shifts the work function until we reach the threshold for 1PPE. The small energy distribution of the emitted electrons at that point minimizes the chromatic aberrations in the real-space PEEM mode, giving rise to very high spatial resolution. In this way we were able to resolve smallest details on the surface with 300 nm resolution in Fig1 (a), even without employing a k-aperture which will improve the base resolution to $< 50 \text{ nm}$. The inset of Fig1 (a) shows a detail selected by the 20 μm field aperture. Beside the Cs-Au(111) results we will show results from our progress towards measuring topological systems like graphene on Ir(111) and Bi_2Te_3 .

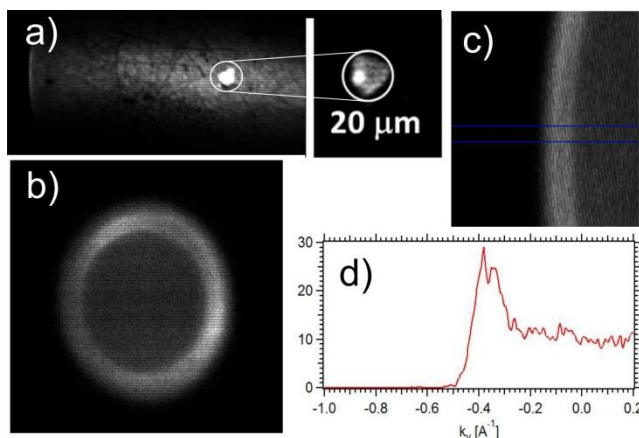


Figure 1: Real space (a) and k-space image (b) of cesiated Au(111) sample. In the case of real space imaging a field aperture enables us to select a specific area on the sample. The spin-splitting in the unoccupied part of the Shockley surface state can be observed in (c) and (d).

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Ultrafast spin polarization control of Dirac Fermions in topological insulators

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Three-dimensional topological insulators (TIs) are characterized by spin-polarized Dirac-cone surface states that are protected from backscattering by time-reversal symmetry. Control of the spin polarization of topological surface states (TSSs) using femtosecond light pulses opens novel perspectives for the generation and manipulation of dissipationless surface spin currents on ultrafast timescales. Using time-, spin-, and angle-resolved spectroscopy, we directly monitor the ultrafast response of the spin polarization of photoexcited TSSs in Sb₂Te₃ to circularly-polarized femtosecond pulses of infrared light. We achieve all-optical switching of the transient out-of-plane spin polarization above the Fermi level, which relaxes in about 1.2 picoseconds. As a result, the dynamics of the generated spin-polarized electrical currents exhibits two distinct timescales for the spin and charge degrees of freedom on the surface (see Figure 1 below). We discuss the mechanisms underlying this behavior. Our observations establish the feasibility of ultrafast optical control of spin-polarized Dirac fermions in TIs and pave the way for novel optospintronic applications at ultimate speeds.

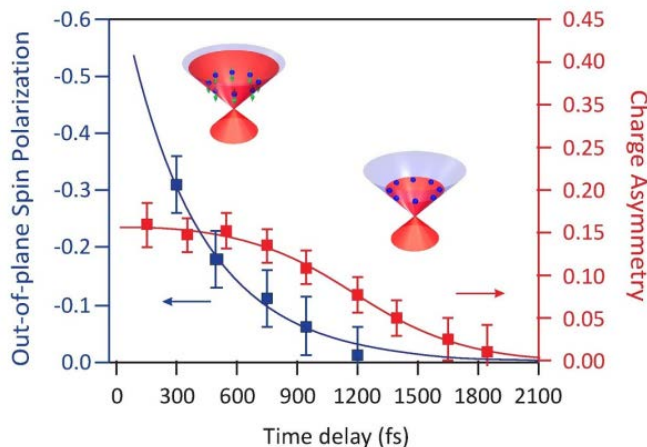


Figure 1. The relaxation dynamics of the net out-of-plane spin polarization (blue) and charge asymmetry (red) exhibits different timescales. The spin polarization relaxes with a time constant of about 0.4 picoseconds, while the charge asymmetry is delayed by about 1 picosecond.

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Odd-frequency Pairing In Topological Superconductivity In A One Dimensional Magnetic Chain

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An array of magnetic chain on top of the superconductor attracts a lot of attention since it can show topological superconductivity which hosts Majorana Fermion (MF) [1]. The experiment of observing of MF has also started [2]. In this study, we have elucidated that MF on the edge of this system coincides with odd-frequency pairing [3]. The concept of odd-frequency pairing naturally arises on introducing the frequency dependence of the pairing function [4]. The odd-frequency pairing ubiquitously exists in inhomogeneous superconducting systems with broken symmetries in, for instance, spin rotation or translation [5].

We have also revealed that the correspondence between the odd-frequency and MF is robust against the distance between magnetic atoms as far as this distance is shorter than the coherence length of the superconductor. Further, we have clarified the close relationship between the pair amplitude of the odd-frequency pair and the direction of the MF spin. These results imply that we can apply the method of detecting odd-frequency pairing to MF. Finally, we suggest the possible experiment for this detection.

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Fig.1. An array of magnetic chain top on the superconductor

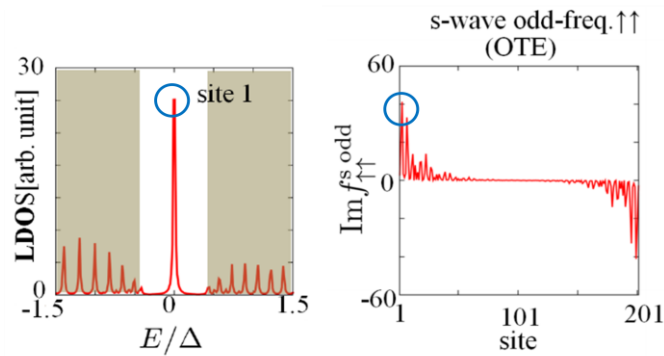


Fig.2.Left: Local density of states on the edge of the magnetic chain
Right: Spatial distribution of the odd-frequency pairing.

Signatures of Twin Grain Boundary Formation in the Band Structure of Bi_2Se_3 Topological Insulator

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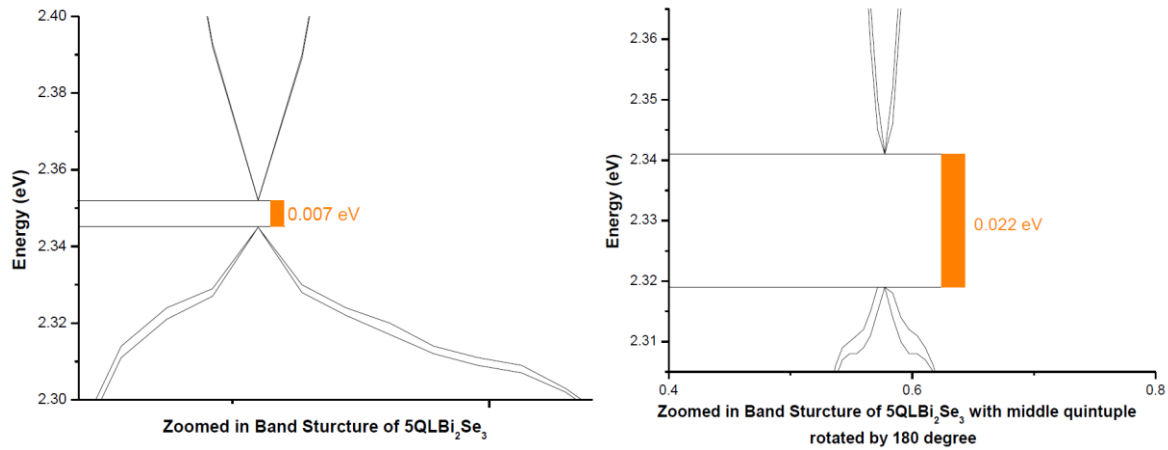
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The formation of different types of defects like grain boundaries, stacking faults and/or vacancies are unavoidable during the growing process of topological insulators (TI) and it is the main reason that limits the use of these materials as spintronic devices[1,2]. Here, we study by means of first principles calculations the impact of twin ($\theta = \pi$) grain boundary (GB) formation on the topological surface states of Bi_2Se_3 slabs.

In particular, we try to answer three different questions: (1) how these GBs or interface states look like[3], (2) how they interact with the topological surface states (mixing of bulk and surface states), and (3), given that these twin boundaries break inversion symmetry, how the electronic structure and the helical spin texture of the surface is modified when displacing the GB from the center of the slab (non-centrosymmetric Bi_2Se_3) to the top/bottom quintuple layer.

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Confined Electron States in Heterostructures based on 3D Topological Insulators (towards a better understanding of the QSHE)

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Three dimensional (3D) topological insulators (TIs) in reduced spatial dimensions have generated prodigious interest since their discovery, because an enhanced surface-to-volume ratio allows one extracting the nontrivial properties of their surface and interface states, which are highly promising for (the) spintronic device applications. Recently the QAH effect has been experimentally discovered in thin films of Cr-doped (Bi,Sb)₂Te₃ magnetic TIs [1].

The 3D TI samples and setups, in reality, occupy only a finite realm of the space and are surrounded generally by other materials. Here we focus on the study of the mechanisms for controlling the quantum transport properties of heterostructures in which the TI film is sandwiched between two convenient insulators. We describe analytically the confined electron states in the thin film. We demonstrate that the Chern numbers of these states are determined by the key ingredients: the interface potential and film thickness. Therefore, if the Fermi level lives within the gap, one could expect the emergence of QSH insulator phase in some region of the parameters. We unveil novel mechanism to influence the topological electron states in the heterostructures based on 3D TI thin films which is responsible for the interface potential driven quantum phase transitions between states with different Chern numbers. We show also that the spectrum and location of the interface/edge electron states in the film exhibit tunability as a function of the effective potential at the interface.

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