O 94: Topology and Symmetry-Protected Materials

Time: Friday 10:30–13:00 Location: GER 38

O 94.1 Fri 10:30 GER 38

Multigap topology and non-Abelian braiding of phonons from first principles — •Bo Peng[1], Adrien Bouhon[1,2], Bartomeu Monserrat[1,3], and Robert-Jan Slager[1] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Nordic Institute for Theoretical Physics (Nordita), Stockholm University and KTH Royal Institute of Technology, Hannes Alfvéns väg 12, Stockholm SE-106 91, Sweden — [3]Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

Non-Abelian braiding of quasiparticles can encode information immune from environmental noise with the potential to realize topological quantum computation. Here we propose that phonons, a bosonic excitation of lattice vibrations, can carry non-Abelian charges in their band structures that can be braided using external stimuli. Taking some earthly abundant materials such as silicates [1] and aluminium oxide [2] as representative examples, we demonstrate that an external electric field or electrostatic doping can give rise to phonon band inversions that induce the redistribution of non-Abelian charges, leading to non-Abelian braiding of phonons. We show that phonons can be a primary platform to study non-Abelian braiding in the reciprocal space, and we expand the toolset to study such braiding processes.

References: [1] Nature Communications 13, 423 (2022). [2] Physical Review B 105, 085115 (2022).

O 94.2 Fri 10:45 GER 38

Electronic Structure of the Weak 3D Topological Insulator $Bi_{12}Rh_3Ag_6I_9$ — •Johannes Hessdörfer[1,2], Eduardo Carillo-Aravena[2,3], Armando Consiglio[2,4], Maximilian Ünzelmann[1], Michael Ruck[2,3], Domenico Di Sante[5], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [3]Anorganische Chemie II, Technische Universität Dresden, Germany — [4]Theoretische Physik I, Universität Würzburg, Germany — [5]University of Bologna, Italy

Weak three-dimensional (3D) topological insulators (TI) can be considered as a stack of 2D TI separated by insulating spacer layers. The first experimentally observed weak TI is $Bi_{14}Rh_3I_9$ [1], in which the TI layers are Kagome nets formed by rhodium centered bismuth cubes. Importantly, a modification of the $[Bi_2I_8]^{2-}$ spacer layer, like e.g. by Ag-substitution, can change the coupling between the 2D-TI and with that decisively influences the topological properties. Here, we investigate $Bi_{12}Rh_3Ag_6I_9$ by means of angle-resolved photoemission experiments and density functional theory band structure calculations. In particular, we will discuss the influence of the modified spacer layer on the electronic structure and compare the results with $Bi_{14}Rh_3I_9$ and other compounds of this family.

[1]Rasche et al., Nat. Mater, 12, 422-425 (2013)

O 94.3 Fri 11:00 GER 38

Doping of coupled 1D topologically protected edge states on the (001) surface of the topological crystalline insulator (Pb,Sn)Se — •Florian Keller, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Lehrstuhl für Experimentelle Physik II, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

Topological crystalline insulators (TCI) are a class of materials with topological protected surface states protected by crystalline symmetry. One representative of this material class is (Pb,Sn)Se which exhibits Dirac fermions at the surface and topologically protected one-dimensional edge state at the step edges with a height equivalent to an odd number of atomic layers [1]. It was shown that the 1D edge states hybridize when two or more odd step edges are in close proximity [2]. The nature of this hybridization indicates that the quasiparticle edge mode is not an infinite quantum 1D state, but is either strongly localized or has a very short coherence length along the edge. One way to check this hypothesis is to increase the coherence length by shifting the Dirac energy close to the Fermi energy [3]. Here we present experiments where Fe adatoms are deposited onto p-doped PbSnSe, resulting in a downwards-bending of the surface band structure. The dependence of the correlation length of Dirac fermions is investigated by determining the edge state hybridization for pristine and doped (Pb,Sn)Se.

[1] P. Sessi *et al.*, Science **354**, 6317 (2016)
[2] J. Jung *et al.*, Phys. Rev. Lett. **126**, 236402 (2021)
[3] P. M. Echenique *et al.*, Surf. Sci. Rep. **52**, 219 (2004)

O 94.4 Fri 11:15 GER 38

Pressure-driven tunable properties of the small-gap chalcopyrite topological quantum material $ZnGeSb_2$: A first-principles study — •Surasree Sadhukhan[1], Banasree Sadhukhan[2], and Sudipta Kanungo[1] — [1]Indian Institute of Technology Goa, 403401 Ponda, India — [2]KTH Royal Institute of Technology, Stockholm

Search for new topological quantum materials is the demand to achieve substantial growth topological phase of matter. In this search process, theoretical prediction is crucial besides the obvious experimental verification. The divination of topological properties in already well-known narrow gap semiconductors are flourishing in quantum material science. We revisited the semiconductor compound in the chalcopyrite series, some of which were potential topological materials. Using this density functional theory-based first-principles calculations, we report a strong topologically nontrivial phase in chalcopyrite $ZnGeSb_2$, which can act as a model system of strained HgTe. The estimates reveal the non-zero topological invariant (Z_2), Dirac cone crossing in the surface spectral functions with spin-momentum locked spin texture. We also report the tunable topological properties from nontrivial to trivial phases under moderate hydrostatic pressure within *7 GPa. A minor modification of a lattice parameter is enough to achieve this topological phase transition easily accomplished in an experimental lab. We have incorporated the discontinuity in the tetragonal distortion of non-centrosymmetric $ZnGeSb_2$ to drive the topological quantum phase transition.

O 94.5 Fri 11:30 GER 38

Shift current in the Haldane model: analytic and numerical evaluation — •Javier Sivianes Castaño and Julen Ibañez Azpiroz — Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain

The shift current is a second order optical response which takes place in noncentrosymmetic crystals and is characterized by a DC photocurrent. As realized recently, the shift current is sensitive to the topology of materials [1]. In particular, DFT calculations have predicted a sign change when going through a topological phase transition (TPT) in the bulk crystals BiTeI and $CsPbI_3$ [2]. Here we analyse the shift current in the Haldane model, as a toy model that describes inversion symmetry breaking and features non-trivial topological phases. We derive a simple analytical expression that accounts for the sign change across the TPT by relating it to the inversion of the mass term, in agreement with Ref [3]. We complement our study by a numerical evaluation on a continuum version on the Haldane model [4]. In this description we study the quantitative importance of the off-diagonal matrix elements of the position operator that are commonly discarded in the tight-binding description.

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[1] T. Morimoto and N. Nagaosa, Sci. Adv. **2**, 5 (2016) [2] L. Z. Tan and A. M. Rappe, PRL **116**, 237402 (2016) [3] Z. Yan, arXiv:1812.02191 [4] J. Ibañez-Azpiroz et al., PRB **92**, 195132 (2015)

O 94.6 Fri 11:45 GER 38

The 2D Ferromagnetic Extension of a Topological Insulator — •Philipp Kagerer[1,2], Celso I. Fornari[1,2], Sebastian Buchberger[1,2], Begmuhammet Geldiyev[1,2], Teresa Tschirner[2,3], Louis Veyrat[2,3,4], Abdul V. Tcakaev[2,4], Martin Kamp[5], Sergio L. Morelhao[6], Vladimir Hinkov[2,4], Hendrik Bentmann[1,2], and Friedrich Reinert[1,2] — [1]Exp. Physik VII, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Leibnitz IFW Dresden — [4]Exp. Physik IV, Universität Würzburg — [5]Physikalisches Institut and RCCM, Universität Würzburg — [6]Instituto de Física, Universidade de São Paulo

3D topological insulators (TI) are known to have a topological nontrivial band structure protected by time reversal symmetry, which also guarantees the metallicity of the surface. Consequently, it is sufficient to break this symmetry only locally at the surface of the sample to gap out the topological surface state (TSS), leading to a variety of novel topological effects, e.g. an axion term in the electromagnetic response and quantized spin-selective edge channels. While most experimental approaches to date have aimed to introduce magnetism globally, we present the first experimental realisation of the *ferromagnetic extension* (1), a design directly interfacing a 3D TI with a two-dimensional non-trivial magnet. Utilizing a single septuple layer $MnBi_2Te_4$ on the prototypical TI Bi_2Te_3, we establish a stable 2D ferromagnetic ground state and introduce a sizeable magnetic exchange gap in the TSS (2).

(1) M.M. Otrokov et al., 2D Mater. **4**, 025082 (2017)
(2) P. Kagerer et al., arXiv 2207.14421 (2022)

O 94.7 Fri 12:00 GER 38

Orbital angular momentum in indenene measured by circular dichroism in ARPES — •Jonas Erhardt, Cedric Schmitt, Simon Moser, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg D- 97074, Germany

Indenene, a monolayer of In atoms arranged in a triangular lattice on SiC(0001), has recently been identified as a quantum spin Hall insulator (QSHI) [1]. Its topological character is encoded in a characteristic energy staggering of its orbital angular momentum (OAM) polarized Dirac states [1]. This makes indenene an ideal test case for recent claims that circular dichroism in angle-resolved photoelectron spectroscopy (CD-ARPES) gives access to local Berry curvature signatures via the OAM [2]. However, a particular challenge of such experiments is the extraction of the intrinsic OAM-related CD signal, requiring its distinction from final state effects and extrinsic contributions induced by experimental geometry.
In this talk, I will present a systematic photon energy dependent CD-ARPES study of indenene's Dirac states and use simple geometric considerations to disentangle experimental from OAM induced CD. The resulting OAM sequence confirms indenene to be a QSHI and thus establishes a new approach to experimentally identify the topological character of a 2D quantum material directly from its bulk states.

[1] M. Bauernfeind *et al.*, Nat. Commun., **12**, 5396 (2021)
[2] M. Schüler *et al.*, Sci. Adv., **6**, 2730 (2020)

O 94.8 Fri 12:15 GER 38

Transfer matrix analysis of non-Hermitian interfaces — •Jacob Fauman — Max Planck Institute for the Science of Light, Erlangen, Germany

Non-Hermitian systems exhibit unique features not present in Hermitian systems, including the so-called non-Hermitian skin effect in which the modes accumulate at the surface of the system. We analyze the interface between a non-Hermitian system and a Weyl semimetal analytically using the transfer matrix method. This approach is especially well-suited to the study of spatially inhomogeneous systems, and allows for analysis of the Fermi arcs at the interface. We also consider the effect of Hermitian and non-Hermitian spectral degeneracies on the interface modes.

O 94.9 Fri 12:30 GER 38

Spectroscopic signatures of non-trivial topology in Weyl semimetals — •Jakub Schusser[1], Hendrik Bentmann[2], Maximilian Ünzelmann[1], Tim Figgemeier[1], Chul-Hee Min[3], Simon K. Moser[4], Jennifer N. Neu[5], Theo Siegrist[6], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, JMU Würzburg — [2]Center for Quantum Spintronics, NTNU Trondheim — [3]Department of Physics, CAU zu Kiel — [4]Exp. Physik IV and Würzburg-Dresden Cluster of Excellence ct.qmat, JMU Würzburg — [5]National High Magnetic Field Laboratory, Tallahassee, Florida — [6]Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Tallahassee, Florida

By performing angle-resolved photoemission spectroscopy (ARPES) on bulk samples we show the spectroscopic manifestation of topological features and Weyl physics beyond the simple photointensity over a broad range of excitation energies from the vacuum ultraviolet to the soft X-Ray regime and compare the surface to the bulk band structure. Our experimental observations were complemented by state-of-the-art first principle photoemission calculations based on one-step model of photoemission. The determinant criterion confirms the arc character of the spoon features in the constant energy contour close to Fermi level in non-centrosymmetric TaP. We further show the drawbacks of the existing spectroscopic techniques used to determine whether the given material has non-zero Chern number and discuss an improved approach for identifying Fermi arcs by the means of differential ARPES measurements as well as the proper final state description.

O 94.10 Fri 12:45 GER 38

Extended Hatano-Nelson model, exceptional points and spectral symmetry — •Julius Gohsrich[1,2], Sharareh Sayyad[1], and Flore K. Kunst[1] — [1]Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Non-Hermitian systems attract a lot of attention in recent years as effective description of open quantum systems. A prominent example in this context is the Hatano-Nelson model. While historically the model has short-range non-reciprocal hoppings, long-range hopping has not been systematically studied. In this talk, I will present our results on the extended Hatano-Nelson model. Using analytical techniques, we demonstrate how the underlying physics of the original Hatano-Nelson model is enriched when longer-range hoppings are also included. I will discuss how the crucial elements of the Hatano-Nelson model, namely, the non-Hermitian skin effect and the exceptional points, are modified for the generalized model.