O 40: Poster: Topological Materials

Time: Tuesday 18:00–20:00 Location: Poster D

O 40.1 Tue 18:00 Poster D

Topological phases of quasi-one-dimensional systems — •Nemanja Madić, Tatjana Vuković, and Saša Dmitrović — University of Belgrade Faculty of Physics, Belgrade, Serbia

Obstructed atomic limits (OALs) of crystalline insulators are topological phases characterized by the Wannier orbitals centers unmovable to ion-occupied positions. Complete information on the orbital's movability from the Wyckoff position (WP) is encoded within the symmetry group of the system. The symmetry of a quasi-one-dimensional (Q1D) system is described by one of the line groups gathered within thirteen infinite families. Their electronic structures are always Wannierizable; consequently, all topological insulating phases of such systems correspond to OALs. As inequivalent topological insulating phases are separated by closing the band gap or breaking the crystalline symmetry, the complete set of such phases can be deduced by analyzing the Q1D systems symmetry group. Here, we explore the OALs of spinless and spinful systems whose symmetry groups belong to the 11th and 13th families. To this end, firstly, the real space invariants, needed to test the movability of Wannier centers allocated at the maximal WP of the line groups, are calculated. Next, these results and recently obtained sets of elementary band representations of ordinary and double line groups are applied to obtain the set of distinct Wannier homotopy classes. Finally, district ion positions of the several systems, with equal symmetry groups, are analyzed to identify all possible phases corresponding to the OAL. Results are illustrated on models created within the PythTB package.

O 40.2 Tue 18:00 Poster D

Topological edge states in quasi-one-dimensional systems — •Bogdan Stanojević and Saša Dmitrović — University of Belgrade Faculty of Physics, Belgrade, Serbia

Robust topological edge states (TESs) of crystalline materials are of great interest, both from the fundamental and application-driven point of view. These states, protected by the lattice symmetry, have been theoretically predicted in 1D inversion symmetric chain [1], as well as in 2D crystals with symmetries p2, p3, and pmm [2]. Here, the analysis is generalized to all quasi-1D (Q1D) systems. These materials are translationally or helically periodic along only one axis, with their symmetry group belonging to one of the thirteen infinite families of line groups (LGs) [3]. Here we consider only time reversal symmetrical Q1D systems. As the full symmetry group of such a system is described by one of the grey LGs, recently derived complete sets of elementary band co-representations (co-EBRs) of grey LG [4], enable the search for TESs: for the system of chosen symmetry, the analytical continuation of distinct elementary band structures at the edges of the irreducible domain singles out possible robust TESs. The results are illustrated on several tight-binding models developed within PythTB package [5].

[1] J. Zak, Phys. Rev. B 32, 2218 (1985). [2] A. Silva, J. van Wezel, SciPost Phys. 10, 137 (2021). [3] M. Damnjanović and I. Milošević, Line Groups in Physics: Theory and Applications to Nanotubes and Polymers (Lecture Notes in Physics vol 801), (Berlin: Springer) (2010). [4] S. Dmitrović S et al., J. Phys. A: Math. Theor. 55 385201 (2022). [5] https://www.physics.rutgers.edu/pythtb/

O 40.3 Tue 18:00 Poster D

On the Edge State of Finite 2D Bi_2Se_3 Crystals — •Auke Vlasblom, Victor Wesselingh, Jesper Moes, Jara Vliem, Daniel Vanmaekelbergh, and Ingmar Swart — Utrecht University, Utrecht, The Netherlands

Topological insulators in two or three dimensions exhibit an insulating bulk, but possess gapless conducting edge or surface states that are protected by time-reversal symmetry. One property of the surface/edge state is spin momentum locking, which results in two types of surface currents, each with opposite spin (up or down) and opposite momentum (direction). In the 2D regime, top and bottom states hybridize and the interior becomes insulating. The two remaining types of edge currents are fully protected from backscattering by non-magnetic impurities.

Here, we study thin (3–6 quintuple layers) finite sized Bi_2Se_3 crystals, prepared via wet-chemical synthesis, using scanning tunneling microscopy and spectroscopy. Measurements are performed on Bi_2Se_3 nanoplatelets with varying thickness to study the transition between 3D and 2D topological insulators. Additionally, the robustness of the edge states is investigated with respect to structural defects and deposition of magnetic impurities.

O 40.4 Tue 18:00 Poster D

Stability of Majorana Fermions in Coulomb-Disordered Topological Insulator Nanowires — •Leonard Kaufhold — Institute for theoretical physics, University of Cologne, Germany

A topological insulator (TI) nanowire, proximity-coupled to an s-wave superconductor (SC) and subject to a longitudinal magnetic field can, in principle, be brought into an effectively spinless superconducting phase under a relatively large region of realistically accessible parameter space and therefore host Majorana Bound States (MBS) at its ends. Due to their non-Abelian statistics, devices that can manifest MBS are a promising candidate for fault-tolerant quantum computing. A TI however, is typically realized as a heavily doped semiconductor with a donor density in the order of $*10^{19}$cm-3. The random potential arising from these impurities by themselves is much larger than the electronic band gap of the surface states due to dielectric confinement, easily destroying their one-dimensional nature necessary exhibit a topologically superconducting phase along the entire wire. Although this potential is screened by the metallic surface states as well as the superconductor, the ultimate fate of the MBS, i.e. whether they can "survive" the screened potential, is not at all obvious. On this poster, we will provide a general review of the TI-SC hybrid nanowire and numerically investigate its phase space based on Andreev spectra, edge state localization and topological invariants.

O 40.5 Tue 18:00 Poster D

A new Bi_4Br_4 surface structure — •Jonathan K. Hofmann[1,2], Hoyeon Jeon[3], Saban M. Hus[3], An-Ping Li[3], Mingqian Zheng[4], Jin-Jian Zhou[5], Zhiwei Wang[4], Yugui Yao[4], F. Stefan Tautz[1,2], Bert Voigtländer[1,2], and Felix Lüpke[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Lehrstuhl für Experimentalphysik IV A, RWTH Aachen University, Germany — [3]Center for Nanophase Materials Science, Oak Ridge National Laboratory, Tennesse, USA — [4]Beijing Key Lab of Nanophotonics and Ultrafine Optoelectronic Systems, Beijing Institute of Technology, China — [5]Institute of Physics, Chinese Academy of Sciences and Beijing National Laboratory for Condensed Matter Physics, China

Bi_4Br_4 is a higher-order topological insulator with a quasi-one dimensional crystal structure [1]. We present a new $Bi_4Br_4(001)$ surface structure analysed with Scanning Tunneling Microscopy/Spectroscopy (STS/STS) at 5 K. STM topography shows an oblique surface structure with characteristic parallel chains shifted by $\sim \frac{b}{3}$ with respect to each other, as opposed to the shift of $\frac{b}{2}$ on α-$Bi_4Br_4(001)$ [1]. We also observe AB-layer stacking, similar to α-Bi_4Br_4 [1]. STS reveals the presence of metallic edge states at surface steps, indicating that this new Bi_4Br_4 structure is also a topological insulator. We propose a crystallographic model for this surface and support our results by density-functional theory calculations.

[1] Shumiya, N.; Hossain, M. S.; Yin, J.-X.; Wang, Z.; Litskevich, M.; Yoon, C.; *et al.*, Nat. Mater. 2022, **21**, 1111*1115.

O 40.6 Tue 18:00 Poster D

The Coarse Geometric Origin of Topological Phases — •Christoph S. Setescak[1] and Matthias Ludewig[2] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Universitätstraße 31, 93080 Regensburg, Germany — [2]Faculty of Mathematics, University of Regensburg, Universitätstraße 31, 93080 Regensburg, Germany

Topological phases of matter rely on the concept that the ensemble of occupied bulk energy bands of a translationally invariant Hamiltonian can be classified by topological invariants by making use of internal electronic symmetries. Non-trivial invariants give rise to exceptional electronic states at the boundary. This approach falls short when dealing with disorder induced by prevalent crystal defects. We propose that one should work in a coarse geometric framework, where the invariant can be defined in the presence of disorder. This construction is physically motivated, provides a natural setting for the bulk-boundary correspondence and furthermore provides a numerical efficient way to calculate the invariants. We apply this approach to a low energy tight-binding model of a three dimensional topological insulator with time reversal symmetry. We discuss the phase diagram in the disorder-free case and analyze the evolution of the topological phase upon the introduction of disorder.