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Warsaw, 16 August 2023

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## **Doctoral dissertation:**

### ***Topological and non-topological boundary states in SnTe and HgTe materials***

#### **Abstract:**

This dissertation focuses on the classification of strong topological insulators and superconductors, gapless topological phases, and higher-order topological phases supporting protected corner states and hinge states. In this thesis, two main research topics were considered. The first topic of our research explored topological boundary states in SnTe. SnTe materials have proven to be highly versatile in investigating the interplay between topology and different types of symmetry-breaking perturbations during the last decade. Our study focused on examining SnTe nanowires under the influence of combinations of a Zeeman field, s-wave superconductivity, and an inversion-symmetry-breaking field. Throughout our research, we successfully revealed the origin of robust corner states and hinge states in the normal state of SnTe. We observed gapless bulk Majorana modes protected by inversion symmetry, leading to quantized thermal conductance in ballistic wires. Additionally, introducing an inversion-symmetry-breaking field caused the bulk Majorana modes to become gapped, resulting in the appearance of topologically protected localized Majorana zero modes at the ends of the nanowire. While we primarily focused on relatively thin nanowires, the observed trends in thickness dependence suggest that realistic nanowire thicknesses could achieve topologically nontrivial phases with experimentally attainable values of the Zeeman field. These findings hold promising possibilities for advancing our understanding and utilization of topological phenomena in SnTe nanowires, and they open up new opportunities for controlling and creating Majorana zero modes by manipulating inversion-symmetry-breaking fields (e.g. via ferroelectricity).

In our second research project, we direct our attention to investigating non-topological boundary states in candidate materials for quantum spin Hall insulators, such as HgTe/CdTe and InAs/GaSb heterostructures. We have observed that these multilayer structures not only host topologically protected helical edge modes but also exhibit additional edge states that can have an impact on scattering and transport, potentially deteriorating the quality of the quantum spin Hall effect. Employing first-principles calculations, we construct an effective tight-binding model for HgTe/CdTe, HgS/CdTe, and InAs/GaSb heterostructures and discover that these materials support extra edge states influenced by the edge termination. The microscopic origin of these additional edge states can be traced back to a minimal model which support flat bands and nontrivial quantum geometry, which gives rise to polarization charges at the edges. As the flat bands interact with each other and other states, when forming the Hamiltonian that describes the entire heterostructure, these polarization charges manifest as the observed additional edge states. Notably, in HgTe/CdTe quantum wells, the additional edge states lie far

from the Fermi level, rendering them inactive in the transport process. However, in HgS/CdTe and InAs/GaSb heterostructures, these states emerge within the bulk energy gap, allowing for the possibility of multimode edge transport. Finally, we demonstrate that since these additional edge modes are non-topological, it is possible to eliminate them from the bulk energy gap by modifying the edge potential, such as using a side gate or chemical doping.

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