

Dipartimento di Fisica



Fantastic topological materials and where to find them:

from computational discovery to materials design



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Room A, building F Via Valerio 2, Trieste



Also on Zoom at https://tinyurl.com/toposeminar Meeting ID: 968 9702 4872 Passcode: topology

In 1988 Haldane (Nobel Prize in Physics 2016) introduced the first model for a topological insulator—the Chern insulator—by considering graphene in the presence of

a staggered magnetic field. In 2005 Kane and Mele realised that by doubling Haldane's model and introducing spins, they could get rid of magnetic fields and obtain a quantum spin Hall insulator (QSHI), i.e. a time-reversal invariant insulator characterised by Z_2 topological order and helical edge states. Since then there has been a significant effort in the study of topological order in real materials.

I will start by introducing our computational screening for novel QSHIs, estimating the relative abundance of these materials in nature. Then, I will present my prediction of monolayer jacutingaite (Pt₂HgSe₃, a naturally-occurring mineral) as the first large-gap Kane-Mele (KM) QSHI. I will discuss the rich physics of monolayer jacutingaite, from its close relationship with graphene to the interplay between spin-orbit coupling, crystal-symmetry breaking, and dielectric response.

Then I will move to bulk jacutingaite, that we discovered to be a dual topological insulator with topologically-protected 001-surface states, as confirmed by ARPES experiments. I will discuss our extension of the KM model to 3D, providing an appealing conceptual framework also relevant for other layered materials made of stacked honeycomb lattices.

Finally, I will present some current efforts on designing van-der-Waals ferroelectric topological insulators.