Electronic Structure Simulations of Novel Quantum Materials for Spintronics and Topological Quantum Computing

Contact: Antimo Marrazzo (Physics Department, University of Trieste)
www.units.it/marrazzo

All materials exist owing to the fundamentals laws of quantum mechanics, but there is a certain class of systems that have been progressively grouped under the umbrella of "**quantum materials**". They include a variety of rather different materials, ranging from high-temperature superconductors, strongly-correlated systems to **topological insulators**, to **Dirac materials** and to the large set of **Van der Waals materials**.

What all quantum materials share is the presence of ***emergent* phenomena** that are responsible for their rather exotic behaviour, posing fascinating scientific questions that deal with the foundations of condensed-matter physics and materials science, such as the existence of emergent particles end excitations like skyrmions, Weyl points, Majorana fermions and many more.

The scientific progress in the field of quantum materials can also contribute substantially to **disruptive changes in modern technology** (see Fig. 1), a prominent example being the rise of **quantum computing**. Most of the quantum computing platforms are enabled by quantum materials with specific properties. Quantum materials promote technologies that are capable of performing tasks that were not accessible before—as in the case of quantum computing—or achieving performance levels that are orders of magnitude larger that could be ever achieved with the current technological paradigms—as in the case of topological electronics.

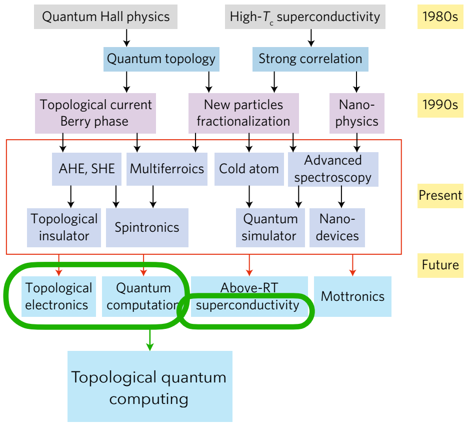

Fig. 1: Brief history of the research on quantum materials and functions, adapted from [6]. The green circles highlight the research areas that intersect towards the field of topological quantum computing.

A compelling case is the proposal of using **2D topological insulators** (a.k.a. **quantum spin Hall insulators** or QSHIs) as a platform for **low-dissipation electronics**. In these materials, while the bulk region remains always insulating, the edge regions are metallic and can host robust dissipation-less electronic transport (see Fig. 2)—even in the presence of rather strong disorder (e.g. impurities or defects)—being protected by the **non-trivial topology** of the bulk electronic wavefunction. In addition, such 1D edge transport can be switched on/off through an external electric field and its spin–momentum locking makes it very promising for **spintronics** functions such as spin-current generators and charge-to-spin convertors.

Fig. 2: The topological quantum "information highway", representing the 1D dissipation-less transport at the edge of a 2D topological insulator, where electrons with opposite spins travel in opposite directions without scattering.

A non-trivial topological state can also coexist with a superconducting state, as in the case of **topological superconductors** (TSC), where **Majorana fermions** emerge as entangled interface states. A pair of Majorana fermions has the degrees of freedom of a single fermion, which is split non-locally in space. The non locality of this "half-fermions" implies that Majorana states are immune to local perturbations, and that is the property that makes Majorana fermions perfect candidates to host **topological qubits**, i.e. qubits that are protected from decoherence due to local noise sources.

In this project, the student will learn how to master cutting-edge electronic structure simulations techniques to study novel quantum materials for spintronics and topological quantum computing applications.

In the process, the student will develop advanced skills in mathematical modelling, numerical simulations, software development and high-performance computing (HPC).