SEMINAIRE ISMO

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First-principles study of the electronic and magnetic properties of topological insulators: doping, alloying

At the end of the last decade, topologically protected states have been observed at the surfaces of the so-called topological insulators (TI), which makes them a subject of intense research. A key characteristic of the aforementioned surface states is their insensitivity to spin-independent scattering, which protects them from backscattering, localization and disorder. These states are potentially useful for spin-based electronics, in which long spin coherence is critical, and also for quantum computing applications, where topological protection can enable fault-tolerant information processing.

In particular binary Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3, are of great interest due to their outstanding structural and electronic properties. These compounds consist of repeated blocks of five atomic layers (quintuple layers, QLs) separated by the van der Waals gaps. Their electronic structure features a narrow band gap and strong spin-orbit coupling, which are responsible for the inverted band structure at the Brillouin zone center and the existence of the topologically protected states. Also, these materials represent promising candidates for thermoelectric applications. Being already well-studied, nowadays these binary TI serve as a basis for new materials or hybrid structures featuring topological properties. This is feasible by stacking of building blocks of different compounds, making heterostructures, specific doping, or surface engineering.

In my talk, after giving a general overview on the physics of topological insulators, I will present part of the current theoretical research of our group in the Max Planck Institute for Microstructure Physics on TI. In particular, electronic and magnetic properties of alloys and magnetically doped binary and ternary TI will be discussed.

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