Topological phase transitions in $MnBi_2Te_4$: an electronic structure view

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Abstract

Topological quantum materials, such as $MnBi_2Te_4$, are of great interest in modern physics due to their unique electronic properties, particularly the presence of topological surface states (TSS) that exist at the boundary between topological and trivial materials. These states are protected by time-reversal symmetry, which prevents electron scattering and makes them highly stable against local perturbations, making such materials promising for applications in quantum computing and spintronics [1]. In magnetic topological insulators, where time-reversal symmetry is broken, new quantum phenomena emerge. This opens the possibility for states such as the quantum anomalous Hall effect and magnetic Weyl semimetals, further broadening the technological potential of these materials [2].

This study investigates the topological phase transitions (TPTs) in the antiferromagnetic topological insulator $MnBi_2Te_4$ using density functional theory (DFT). It focuses on how variations in spin-orbit coupling (SOC) affect the electronic and spin structures of $MnBi_2Te_4$. At the critical point of the TPT, the bulk band gap and the Dirac point gap in the TSS reach their minimum as the SOC strength decreases. Beyond this point, the bulk band gap increases as the system transitions to a trivial state, accompanied by an inversion of the Bi-pz and Te-pz orbital states and a corresponding inversion of spin polarization in the Dirac cone.

Doping $MnBi_2Te_4$ with Sn or Ge produces a similar effect. Changes in the spin-orbit interaction and interlayer coupling caused by doping result in a non-linear dependence of the gap on the concentration of Sn or Ge. Like the SOC variation, the bulk band gap initially decreases and then increases as the system transitions to a trivial state, also accompanied by the Bi-pz and Te-pz orbital state inversion. These findings show that doping can control topological phase transitions similarly to SOC variation, with orbital contributions playing a key role.

Additionally, the study explores how magnetic ordering and SOC tuning can produce different electronic phases. In the ferromagnetic (FM) phase, $MnBi_2Te_4$ transitions from a topological insulator (TI) to a Dirac semimetal (DSM), then to a Weyl semimetal (WSM), and finally back to DSM before reaching the trivial insulator (TrivIns) state. In the antiferromagnetic (AFM) phase, the system transitions directly from an AFM TI to a TrivIns state via a single-point transition through the DSM phase.

These findings highlight the potential of $MnBi_2Te_4$ for studying exotic quantum phenomena and its promising applications in spintronics and quantum computing.

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Bibliography

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