# FIRST PRINCIPLES INVESTIGATIONS OF MAGNETICALLY DOPED TOPOLOGICAL INSULATORS AND FERROELECTRIC MATERIALS

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## Abstract

Topological insulators are promising materials for future spintronic applications due to the unique properties of their spin-polarized surface states. Three-dimensional topological insulators (TIs) are characterized by spin-polarized Dirac-cone surface states that are protected from backscattering by time-reversal symmetry. Typical example of so called 3D topological material is $Bi_2Se_3$. Even though, bulk of this material is showing semi-conducting properties, its surface is metallic, as is shown on the Fig 1.

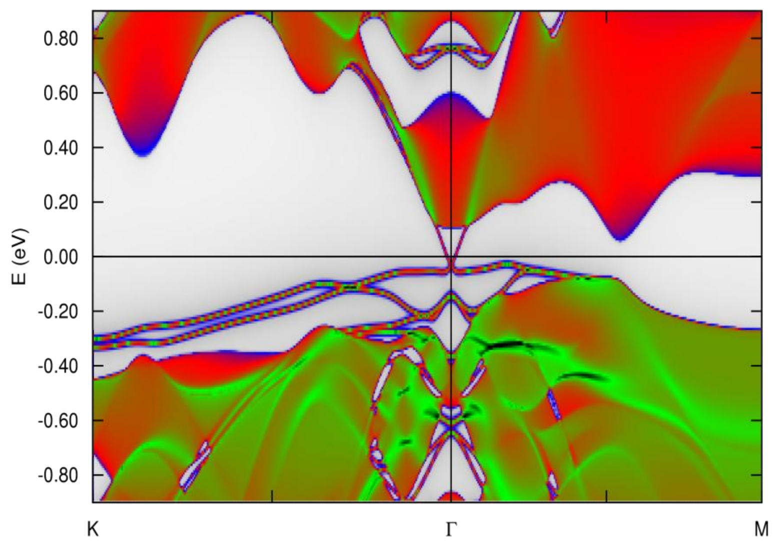


Fig. 1: *Spectral function of semi infinite $Bi_2Se_3$(111) surface, showing typical topological surface states with Dirac like point at the Gamma point*.

There are several ways how to manipulate the spin polarisation of the topological surface state. One of them is the control of the spin polarization of topological surface states (TSSs) using femtosecond light pulses opens novel perspectives for the generation and manipulation of dissipation less surface spin currents on ultrafast time scales. Using time-, spin-, and angleresolved spectroscopy, we directly monitor the ultrafast response of the spin polarization of photoexcited TSSs to circularly polarized femtosecond pulses of infrared light. By means of the one step model of photoemission, these experiments can be studied in a detail. Here we show in particular newly found surface resonances and their effects on the spin relaxation processes [1,2,3].

In addition to these experiments, the topological protected surface state can be manipulated by magnetic doping. Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped $Bi_2Se_3$ band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [4] as well as XAS and XMCD [5] experimental data**.**

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