Spin-resolved and temperature dependent electrical transport properties of topological insulators from the first principles

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Topological insulators (TI) exhibit wide range of interesting phenomena connected to their surface states. Huge amount of both theoretical or experimental studies have been dedicated to this topic; however, bulk states of the TI are of extreme importance and are closely connected to the topological properties of the TI.

We will introduce fully relativistic ab initio calculations with temperature dependence suitable to describe real behavior of TI and other materials as needed in applications. Description of spin-resolved electrical conductivity will be also presented; it opens possibility to investigate possible applications of TI in spintronics.

Calculations from the first principles taking into account chemical and temperature disorder will be used in order to describe robustness of the TI in the presence of impurities or phonons. Finite temperature may dramatically influence behavior of investigated systems; however, most of the calculations are usually being done at zero temperature. Fig. 1 shows an example of huge change of electrical resistivity of a pure and Te-rich topological insulator Bi$_2$$_x$Te$_{3+x}$ for wide range of temperatures and it demonstrates that the insulating character of the bulk material strongly depends on both chemical and temperature disorder which may present a huge complication for applications in real devices.

Electrical transport properties are investigated using computational codes based on the Dirac equations with the tight-binding linear muffin-tin orbital (TB-LMTO) method and coherent potential approximation (CPA) \cite{1}. Theoretical approach to calculate relevant physical phenomena, especially electrical transport properties, from the first principles in a wide thermal range is developed. Frozen phonons are represented by shifts of nuclei from their equilibrium positions using linear transformation of LMTO potential functions \cite{2}. Discussion of proper selection of displacement vectors (directions and magnitudes of displacements for the nuclei) will be included. Methods describing finite temperatures have been tested on transition metals and simple alloys \cite{2} and may be used for topological insulators as well.
Figure 1: Temperature dependence of electrical resistivity for Te-rich topological insulator Bi$_{2-x}$Te$_{3+x}$. The pure material ($x_{Te}=0$) is insulating at low temperatures; however, even slightly increasing concentration of Te changes the resistivity dramatically.
