Referee report

on Ph.D. thesis

Topological insulators and magnetic order

written by Mgr. Jakub Šebesta

The Ph.D. thesis of Mgr. Jakub Šebesta mainly focuses on theoretical description 3D topological insulator Bi_2Se_3 and its topological properties. Namely, the first part of the thesis nicely introduces DFT technique to describe electronic structure in solids, followed by introduction to magnetic properties of solids. Next chapter introduces topological properties of solids, such as Berry curvature, electronic topological surface states and topological invariants. This theoretic introduction is followed by electronic and crystallographic structure of BiSb and Bi_2Se_3 crystals. The study follows by introducing Mn into Bi_2Se_3, providing magnetic properties of the compound. The magnetic properties are calculated in form of saturation magnetization, Curie temperature and exchange interactions, and expressed its dependence on Mn crystallographic positions and crystallographic ordering in general. The amount of calculations is impressive and non-trivial. Last chapter of the thesis presents electronic structure of thin-films of Bi_2Se_3, separated by vacuum. It allows to calculate ab-initio the electron's surface states and related topological Dirac points, which I found very interesting.

Each of those chapters provides very interesting and current topics as demonstrated by authors publications in prestigious journals (Nanomaterials, Phys. Rev. B, Phys. Rev. Materials). I consider the thesis to be very well and clearly written, with minima of mistakes and typos. I suggest the thesis to be accepted for the Ph.D. defense.

Topics to discussion:

- Spin orbit interaction is usually described by perturbative approach. In chapter 6, the difference between exchange interactions calculated by perturbative and full relativistic spin-orbit coupling are compared, suggesting only small influence of the way how spin-orbit coupling is introduced. How does the energy of electrons (or electronic structure) in Bi_2Se_3 changes when using different approaches to describe spin-orbit coupling?

- Exchange interaction in Bi_2Se_3 calculated in section 5.3. shows that the strongest exchange (Fig. 5.12) is not with the nearest neighbor, but with the second-nearest neighbor., which I found interesting. Also, what breaks the symmetry of the exchange interaction, being three-fold, not six-fold as the crystal structure. Is there some simple view?

- Chapter 7 describes the electronic structure of Bi_2Se_3 surface states, using projected Bloch spectral function (BSF). As electronic structure calculation are done in k-space, how does the spatial sensitivity to separate the surface states works? Also, what is the physical meaning of intensity of BSF (e.g. Figs. 7.2-7.3).

Prague, March 1, 2021

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