Referee review report on the PhD thesis of Libor Šmejkal:

"Topological band theory of relativistic spintronics in antiferromagnets"

This thesis comprises the results of theoretical and computational work in a field of band and transport theory of the topologically non-trivial solids with emphasis on the metal-insulator transition (MIT) and the Hall effect in the anti-ferromagnets. The thesis consists of four chapters, and is based on eleven publications in peer review journals. The results of the thesis are of the high scientific quality.

I have a few comments regarding the presentation of the results:

The Chapter 1. describes the magnetic symmetry analysis, the topological properties of the wavefunctions, and the concepts of the transport theory for the anti-ferromagnets. It is written in a form of review which is more appropriate to the research paper. I would expect more basic introduction including the details, like analytical derivations etc., which are usually missing in the research papers.

The Chapter 2. is devoted to the relativistic band theory. Overall description of the relativistic density functional theory is formal and incomplete, and misses important points. The DFT+U version is presented in the spherically-symmetric form that is not compatible with the calculations which include the spin-orbit coupling. The subsection **"**Computational scheme**"** together with description of the calls of the computer routines belong to the appendix rather to the main text.

The Chapter 3. describes the applications of the theory outlined in Chapters 1. and 2. to the MIT in CuMnAs, the anisotropic magnetoresistance (AMR) in NiMnSb ferromagnet, and Mn2Au anti-ferromagnet. What I am missing is the calculations and analysis of the magneto-crystalline anisotropy in relation to the AMR.

The Chapter 4. is devoted to Dzyaloshinskii - Moria interaction (DMI) and spontaneous Hall effect and in RuO2, IrMn3, Mn3Sn, and CoNb3S6. The symmetry considerations for the Hall effect in the anti-ferromagnets are given. The DMI and the spin canting in non-collinear anti-ferromagnets are described. The phenomenology of the effect is very well introduced. The suggestions are made for experimental verification of this effect.

Finally, I would like to poit out that the Ref. 148 is incorrect.

My specific quastions to the author are:

1. What is the reason that the relativistic energy functional in Eq. (2.10) is reduced to the form which includes the **(σ B)** form? Is it the only technical issue or there is a fundamental difficulty to work directly with the vector-potential **A** in Eq. (2.10)?
2. Are there the magneto-crystalline anisotropy calculations for CuMnAs and Mn2Au? Is there a relation to AMR?
3. Was the the so-called Dudarev parametrization for the DFT+U used for RuO2 calculations with VASP? Where the electronic structure results of VASP verified with ELK for RuO2?

In summary, the work of Mr. Šmejkal is very impressive and of the high scientific quality. Importantly, his work is linked directly to the experimental research, and has a potential for applications in the modern technology. The author demonstrated ability to conduct high quality scientific work, to collaborate and work as a member of the world-leading research team, and to carry on his independent research.

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