Magnetic Symmetry Analysis and Ab-ititio Calculation of Anomalous Hall Conductivity in Co_2TiSn

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Abstract: It has been known that the full-Heusler Co2TiSn is a promising half-metallic material for spintronics devices with high spin polarization at the Fermi energy and the high T_c [R. Ooka,*et al.*, IEEE Magn. Lett. **8** 3101604 (2017); P. J. Webster and K. R. A. Ziebeck, J. Phys. Chem. Solids **34**, 1647 (1973)]. In addition, recently it has been found to be a magnetic topological "Weyl semimetal", which carries topological charge at the Weyl points in the reciprocal space and shows finite anomalous Hall conductivity (AHC) [G. Chang, *et al.*, Sci. Rep.**6**, 38839 (2016)]. Several works have been done so far for exploring new magnetic Weyl semimetal with both collinear- and non-collinear spin ordering [Nayak *et al.*, Sci. Adv.; 2:e1501870 15 April 2016]. In our study, in order to understand the microscopic mechanism of the AHC, first we perform symmetry analysis of magnetic configurations in Heusler compounds considering symmetry of Berry curvature in the reciprocal space [M.-T. Suzuki, T.Koretsune, M. Ochi, and R. Arita, Phys.Rev. B **95**, 094406(2017)], and then seek several magnetic configurations which allows finite AHC. To confirm the symmetry analysis, we carry out *ab-initio* calculations with Wannier-function interpolation scheme to evaluate AHC for each magnetic configuration. We discuss the electronic structure and the mechanism of large AHC in Co_2TiSn $(X = Si, Ge, Sn)$ as well as a strategy to enhance the AHC in Heusler compounds.

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