Role of Chemical Disorder in Tuning the Weyl Points in Vanadium Doped Co_2TiSn

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Abstract. The lack of time-reversal symmetry and Weyl fermions give exotic transport properties to Co-based Heusler alloys. In the present study, we have investigated the role of chemical disorder on the variation of Weyl points in Co2Ti1−xVxSn magnetic Weyl semimetal candidate. We employ the first principle approach to track the evolution of the nodal lines responsible for the appearance of Weyl node in Co_2TiSn as a function of V substitution in place of Ti. By increasing the V concentration in place of Ti, the nodal line moves toward Fermi level and remains at Fermi level around the middle composition. Further increase of the V content, leads shifting of nodal line away from Fermi level. Density of states calculation shows half-metallic behavior for the entire range of composition. The magnetic moment on each Co atom as a function of V concentration increases linearly up to x = 0.4, and after that, it starts decreasing. We also investigated the evolution of the Weyl nodes and Fermi arcs with chemical doping.

The first-principles calculations reveal that via replacing almost half of the Ti with V, the intrinsic anomalous Hall conductivity increased twice as compared to the undoped composition. Our results indicate that the composition close to the 50% V doped Co_2TiSn will be an ideal composition for the experimental investigation of Weyl physics.