

Disorder-induced topological properties in CoFeCrZ (Z = Al and Ga) Heusler alloys: From spin gapless semiconductor to magnetic Weyl semimetal

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Supplementary information

In B2-type structure, Cr and Z atoms randomly occupy the crystallographic $4b$ ($1/2, 1/2, 1/2$) and $4a$ ($0, 0, 0$) sites. The unit cell contains four interpenetrating FCC sublattices with each atomic species occupying one sublattice. To model the disorder, two Cr atoms from the $4b$ sites were interchanged with two Z atoms from the $4a$ sites. Since each site has four equivalent atomic positions, multiple configurations are possible. We tested several configurations for CoFeCrAl and found only minor variations in the positions of the Weyl points. Fig. S1 shows the configuration used in this work as B2-type structure. To keep the calculations simple (less time consuming), we have used unit cell for all the calculations.

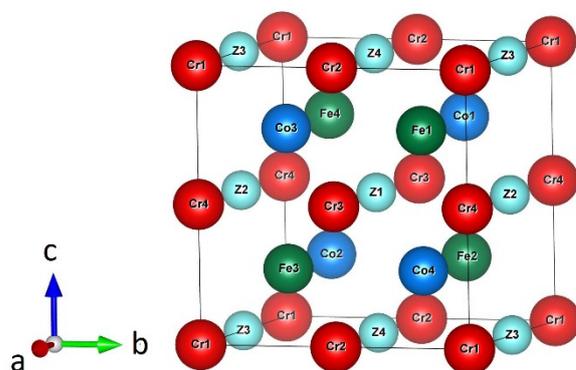


Fig. S1 B2-type structure obtained by interchanging two Cr atoms from the $4b$ sites with two Z atoms from the $4a$ sites (Z = Al / Ga).

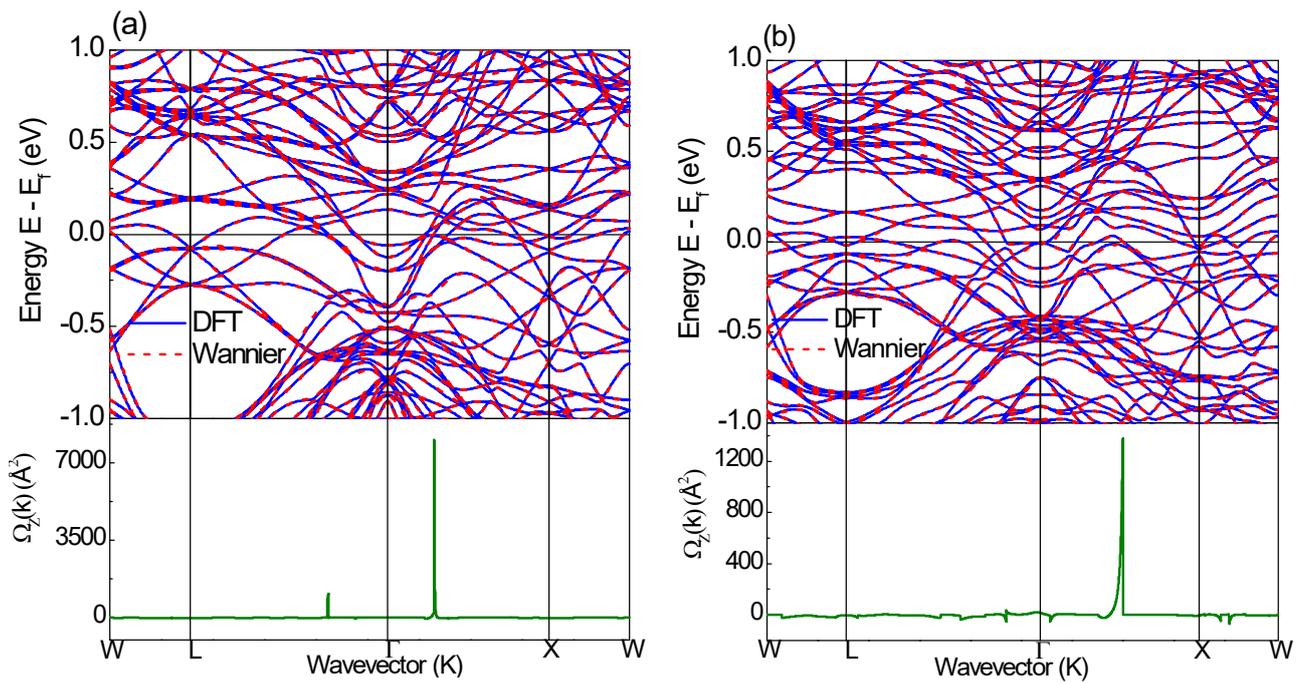


Fig. S2 Top: Band structure obtained from density functional theory and Wannier interpolation with spin-orbit coupling for B2 disordered (a) CoFeCrAl and (b) CoFeCrGa. The blue line shows the DFT bands while red dash line shows the Wannier interpolated bands. Bottom: Berry curvature along the high symmetry path.

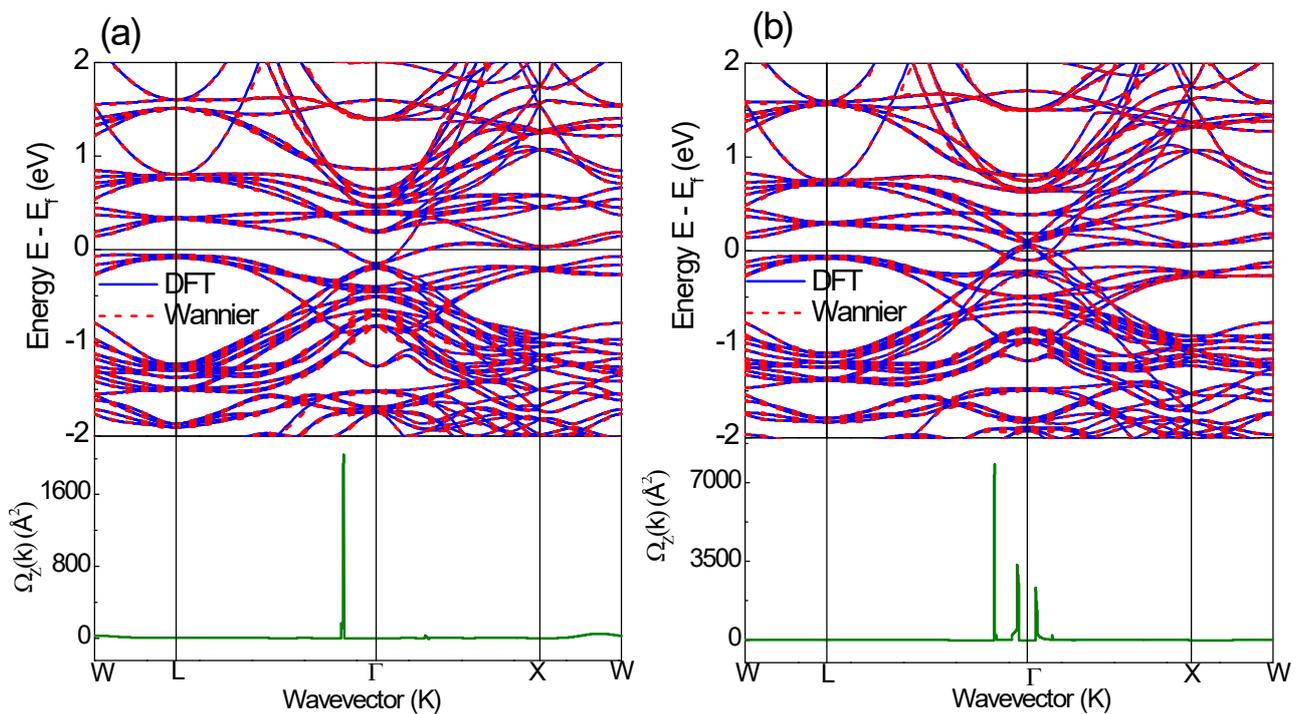
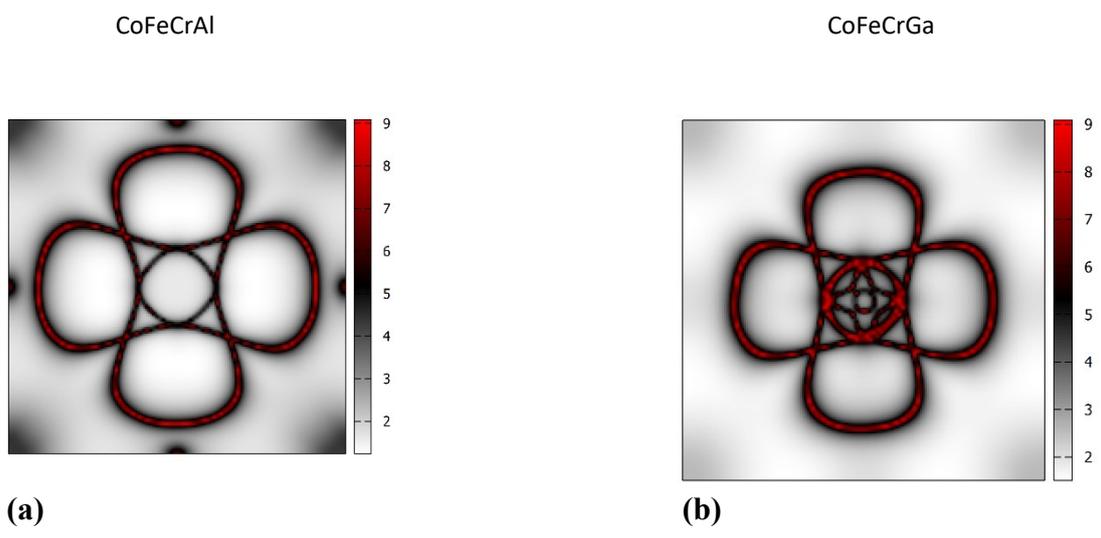


Fig. S3 Top: Band structure obtained from density functional theory and Wannier interpolation with spin-orbit coupling for ordered (a) CoFeCrAl and (b) CoFeCrGa. The blue line shows the DFT bands while red dash line shows the Wannier interpolated bands. Bottom: Berry curvature along the high symmetry path.



(c)

(d)

Fig. S4 The bulk planar Fermi surface with SOC for ordered (a) CoFeCrAl, (b) CoFeCrGa, B2 disordered (c) CoFeCrAl and (d) CoFeCrGa. The color bar indicates the spectrum intensity in arbitrary units. Red color indicated the energy bands contributing to the Fermi surface.

