Supplemental Material: Co-emergence of Dirac and multi-Weyl Topological Excitations in Pnictide Antiperovskites

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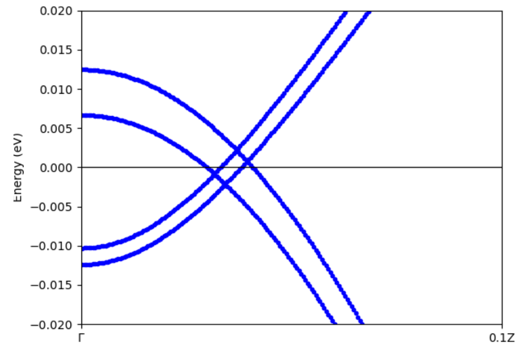
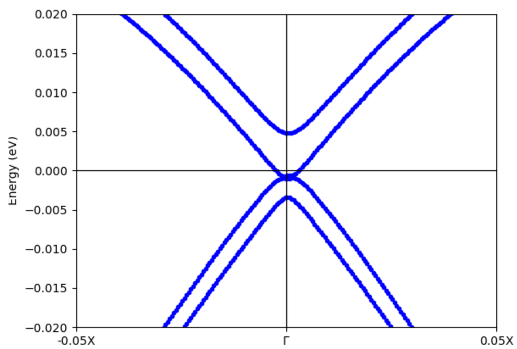
EXPLICIT VIEW OF MULTI-WEYL CHARACTER

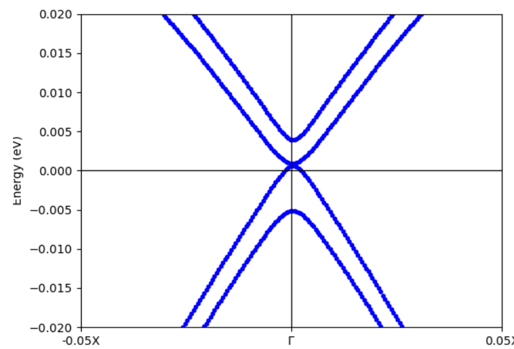
A set of hopping amplitudes was obtained from Wannier functions based on 48 atomic orbitals, viz. Bi 6p, P 3p, Ca $4s, 3d$. The 4 bands crossings along Γ-Z as shown in Fig. 1a are reproduced by hopping amplitudes extendinng to nine neighbour unit cells. Fig. 1b-1e show energy dipersion *perpendicular* to $\hat{z}$ for each of the four degenerate points, where two are seen to be multi-Weyls (Fig. 1b and 1c), *i.e.* dispersion is linear along $\hat{z}$ but quadratic in directions perpendicular to $\hat{z}$. This behavior is also seen in other Dirac semimetals, eg. Na_3Bi. The tight binding scheme can be extended to obtained a 4×4 model Hamiltonian through $k \cdot p$ expansion at Γ point. However, since the Weyl points do not occur at small k, such an abbreviated expansion cannot reproduce a realiable description for the band crossings.



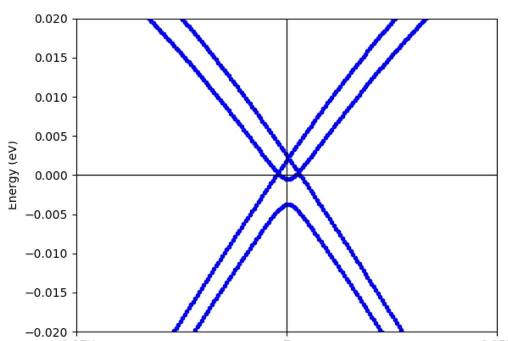
(a) Band crossings along Γ-Z



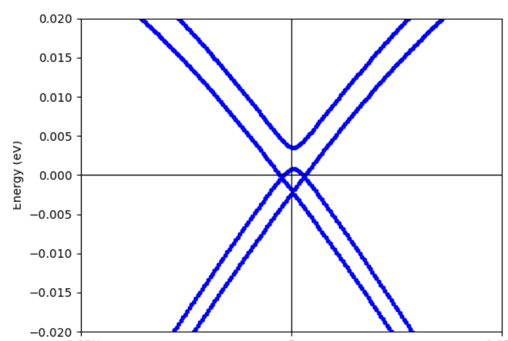
(b) Left point



(c) Right point



(d) Top point



(e) Bottom point

FIG. 1: Band structures obtained from the hopping-parameters up to nine neighbouring cells (six is minimum number of cells for the resulting bands to be reasonable). (a) The energy bands along Γ-Z shows four degenerate points where two are multi-Weyl points. (b)-(e) Energy dispersion perpendicular to $\hat{z}$ at $k_{z,j} = 0.032$ (left point), 0.039 (right point), 0.037 (bottom point) and 0.034 (top point), in units of $(\frac{\pi}{c})$.