Prediction of a new type-I antiferromagnetic Weyl semimetal in the full-Heusler compound InMnTi2

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Topological materials have been one of the main focus of studies in the past decade due to their topologically protected properties that can be exploited for the fabrication of new devices. Weyl semimetals are a class of topological semimetals with non-trivial linear band crossing close to the Fermi level. The existence of such crossings gives rise to low energy properties akin to a Weyl fermion and is responsible for the exotic physical properties. In order for these crossings to exist, either time-reversal or inversion symmetry or inversion must be broken, the latter being the favored one from an experimental point of view, but leading to more complex electronic properties.

In this work we show the properties computed through ab-initio methods for InMnTi2, a newly proposed inversion-breaking Weyl semimetal. We show results derived both through density functional theory and through Wannier interpolation. This material shows several feature that are comparatively more intriguing with respect to other known inversion-breaking Weyl semimetals such as the transition metal monopnictides. Mainly the distance between two neighboring nodes is large enough to observe a wide range of linear dispersion in the band. Moreover only one kind of such pair of nodes can be distinguished in the Brillouin zone. Finally the lack of other trivial points makes it so the low-energy properties of the material can be directly related to the presence of the Weyl nodes and the other transition mental monopnictides. Nevertheless, while much easier to realize, these kind of WSs present a much more complicated band structure landscape. First, in a inversion-breaking WS nodes are present in a number of pairs multiple of 4. Another complication is the proximity of two neighboring nodes in the same pair which causes a distortion of the usually linear dispersion. Finally, the more complicated band structure can give rise to the presence of many trivial points, which have been shown to give a non-negligible contribution to the low-energy optoelectronic properties of the material.

In this work, we perform a systematic study of the properties of InMnTi2, a non-centrosymmetric antiferromagnetic full-Heusler compound, belonging to the space group 216. Given the lack of inversion symmetry, we expect to find Weyl nodes organized in 4n pairs. Indeed, from our analysis, we find 12 pairs of equivalent type nodes throughout the entire BZ of the material. Our studies show that the distance between a pair of neighboring nodes is greater than that of the transition metal monopnictides. Finally we also find that trivial point are not present, as the only fermi pockets are given by the WNs.

I. INTRODUCTION

Topological semimetals constitute a class of materials, where protected band crossings occur. They can be distinguished in either Dirac semimetals or Weyl semimetals when the crossings happens at isolated nodes in the Brillouin zone (BZ), or nodal line semimetals when the crossings spans an entire line. The nodes can be distinguished into Dirac or Weyl using their description within a $k \cdot p$ framework which can take the form of either a Dirac or a Weyl Hamiltonian. The former describes a fourfold degenerate crossings with no chirality, while the latter describes a pair of twofold degenerate crossings with opposite chirality, as guaranteed by the fermion doubling theorem. The presence of these nodes lead to the definition of a quasi-particle with behavior similar to a Dirac or Weyl fermion respectively. The focus of this paper will be on WSs that exhibit a wide range of interesting properties such as the Adler-Bell-Jackiw anomaly which leads to the observation of negative magneto-transport and the presence of atypical surface states known as Fermi arcs. WSSs have hence been proposed for many applications ranging from the realization of qbits to Veselago lenses and lasing.

One of the main requisite for the realization of a WS is the breaking of either time-reversal or inversion symmetry. If both are present at the same time, it can be shown that two nodes with opposite chirality will always be degenerate giving rise to a four-fold topologically trivial crossing. While TR-breaking WSs are easier to deal with from a purely theoretical framework, given that they can exhibit only a single pair of Weyl nodes (WNs), they are in practice difficult to realize. A major breakthrough in the study of WSs was achieved with the experimental realization of the inversion breaking WS TaAs and the other transition mental monopnictides. Nevertheless, while much easier to realize, these kind of WSs present a much more complicated band structure landscape. First, in a inversion-breaking WS nodes are present in a number of pairs multiple of 4. Another complication is the proximity of two neighboring nodes in the same pair which causes a distortion of the usually linear dispersion. Finally, the more complicated band structure can give rise to the presence of many trivial points, which have been shown to give a non-negligible contribution to the low-energy optoelectronic properties of the material.

II. METHODS

The density functional theory (DFT) calculations in this work have been carried out using the open-source plane wave code Quantum ESPRESSO in combination with the norm-conserving full-relativistic pseudopotentials from the ONCVPSP library with the exchange and correlation functional derived within the Perdew, Burke and Ernzerhof-generalized gradient approximation. The parameters and convergence
thresholds set for this calculations are higher than the conventional ones in order to guarantee an accuracy of the order of 1 meV for the resulting eigenvalues. In particular we make use of a cutoff for the wavefunctions G-vectors of 150 Ry. The initial self-consistent calculation is carried out on a $9 \times 9 \times 9$ Monkhorst-Pack mesh. Successively nscf calculation on a $12 \times 12 \times 12$ grid has been used as the base to perform the wannierization of the wavefunctions with Wannier90. In order to determine the magnetic configuration of the material, several supercells have been considered, with different starting spin configurations. For the Hubbard correction, we employed Dudarev’s rotationally-invariant scheme with values of $U$ of 2.45 eV and 2.27 eV for the Mn and Ti atoms respectively, which have been calculated using perturbation theory fully including spin-orbit corrections with a $4 \times 4 \times 4$ $\mathbf{q}$-points mesh. The bands used for the wannierization have been chosen so as to include the entire isolated manifold including both the valence and conduction bands around the Fermi level. Following the wannierization of the wavefunctions, WannierTools has been employed in order to perform a Wannier interpolation on a denser $151 \times 151 \times 151$ k-point mesh. Such grid has been used for the calculation of the Fermi surface, density of states (DOS). The iterative Green’s function method is used in order to compute the surface states on a tetragonal supercell. The surface is cut along the [001] direction and the states are computed both for the Ti/Mn- and In-terminated surfaces.

The Berry curvature ($\Omega$) defined as the rotor of the Berry connection ($A$)

\begin{equation}
A_n(k) = i \langle u_{nk} | \nabla_k | u_{nk} \rangle,
\end{equation}

\begin{equation}
\Omega_n(k) = \nabla_k \times A_n(k)
\end{equation}

has been computed using WannierBerri. The Chern number of the nodes has been computed, both by considering the flux of $\Omega$ on a sphere surrounding the node, and using Z2pack which tracks the evolution of the hybrid Wannier charge centers (HWCCs).

\begin{equation}
C = \int_{BZ} dS \cdot \Omega_n(k)
\end{equation}

The frequency-dependent dielectric tensor $\epsilon_{ij}(\omega)$ is calculated within the independent-particle approach. The imaginary part of the diagonal elements ($j = x, y, z$) is given as

\begin{equation}
\text{Im} \epsilon_{jj}(\omega) = \left( \frac{2\pi e}{m_0} \right)^2 \frac{1}{V} \sum_{\mathbf{k}} \sum_{c,v} \left[ f(\epsilon_v(\mathbf{k})) - f(\epsilon_c(\mathbf{k})) \right] \\
\times |\langle \mathbf{p}_j | \mathbf{e}_c | \mathbf{e}_v \rangle|^2 \delta(\epsilon_c(\mathbf{k}) - \epsilon_v(\mathbf{k}) - \hbar \omega)
\end{equation}

In order to obtain higher accuracy for the low-energy, a combination of an anti-cropped $54 \times 54 \times 54$ and a cropped $218 \times 218 \times 218$ has been used. The crop(anti) has been performed by taking all the k-points within(outside) a sphere of radius 0.05 Å centered on each WN. The results from the two calculations have been then merged by taking into account the weight of the k-points involved. The optical conductivity can be calculated from the dielectric tensor using the formula

\begin{equation}
\text{Re} \sigma_{jj}(\omega) = \frac{\omega}{4\pi} \text{Im} \epsilon_{jj}(\omega)
\end{equation}

The entire process has been automated by writing workflows using AiiDA, which let us keep track of the metadata and provenance for every step of the calculation. The relative plugins for QE and Z2pack have also been employed.

III. RESULTS AND DISCUSSIONS

When testing the magnetic configuration of the material, even when considering supercells, the non-magnetic one results as the most energetically favored. Conversely, when the Hubbard correction is taken into account, the state converges to an antiferromagnetic one, that can be obtained by considering only one cell. This happens because the Ti and Mn atoms form 2 sublattices with opposite spin configuration. Notably, in the work of Shi et al, where they study an equivalent inverted Heusler compound Ti$_2$MnAl, they also obtained an antiferromagnetic configuration as the most stable one, with opposite spin direction on Ti and Mn sublattices, but without the need to include the Hubbard correction. The band dispersion of the material have been computed both in a non-magnetic configuration and, at the antiferromagnetic one (see Fig. 1). For the non-magnetic calculations, a near-linear crossing can be observed along the $\Gamma \rightarrow K$ direction, due to the presence of the Weyl nodes in its proximity. In the antiferromagnetic configuration, a wider direct gap appears along the same line, closer to the $K$ point. This happens because the the pair of nodes is closer the the $K$ point, but the distance of the nodes within the pair is also greater, hence the single nodes are further away from the high-symmetry line. For both configurations, 12 pairs of nodes appears, that are all equivalent by symmetry in the non-magnetic case, while for the antiferromagnetic one, they are subject to a a Chern and K dependent shift. This is expected as it is known that the position of a Weyl node can be shifted due to a magnetic field. It can be seen from Fig. 1 that the nodes on the $k_z = 0$ plane are shifted upward/downward if their chirality is -1/+1. For both configuration, the computed Fermi surface is similar, hence we report only the antiferromagnetic one in Fig. 1. From this image we can see that the Fermi surface forms closed pockets around the nodes, a distinctive feature of a type-I semimetal. The lack of other pockets in the BZ also indicates that the only contribution to the low-energy property will be from the dispersion around the Weyl nodes, hence no ”trivial points” can be identified in the material. For comparison, transition metal monopnictides such as TaAs exhibit trivial pockets of both hole
FIG. 1: (a) Plot of the BZ including the position of the WNs in the antiferromagnetic configuration. The nodes with chirality +1 are shown in red, while the one with chirality -1 are shown in blue. The green lines show the high-symmetry path on which the bands have been calculated. (b) Plot of the Fermi surface taken from a Wannier interpolation on a 151 × 151 × 151 k-point grid in the antiferromagnetic configuration. The Fermi surface shows pockets only surrounding the 12 pairs of WNs. It is interesting to node the absence of other pockets of Fermi surface which shows for the absence of trivia points. (c) Band structure along the high-symmetry path computed from DFT for the antiferromagnetic(red) and non-magnetic(dashed blue) configurations.

FIG. 2: Plot of the DOS near the Fermi level computed from a Wannier interpolation on a 151 × 151 × 151 k-point grid with a gaussian smearing of 1 meV. The inset shows a zoom in an energy range closer to the Fermi level. In green the fit of the DOS near the WN using a quadratic polynomial. The DOS goes to zero near -0.096 meV which is the expected position of the WNs with respect to the Fermi level. This indicates that no other states are present near the Fermi level, but those that form the nodes.

and electrons across their BZ. This constitutes an important result given that the presence of trivial points in a WS can often completely mask its Weyl properties for optoelectronic applications. Notably, when analyzing the character of the pockets, given the position of the nodes in the energy space, which is −79 meV (+60 meV) for the antiferro(non-)magnetic configuration, in the non-magnetic configuration they come out as hole pockets, while in the antiferromagnetic one they are electron pockets. This show that while topology is very robust and not destroyed by adding an antiferromagnetic spin configuration, this effect is still required to correctly assess the properties of the nodes.

The lack of trivial nodes can also be inferred by analyzing the DOS of the material shown in Fig. 2. Given a three-dimensional WN, from ref. we can see that in such a region, the expected behavior of the DOS should be \( D(E) \sim (E - E_W)^2 \). A fit with a quadratic polynomial is also shown in the inset of Fig. 2 which overlap perfectly with the results computed ab-initio. This, together with the fact that the DOS goes zero at \( E_W \) (within the limits of the broadening used), is another indication that trivial points are not present and the low-energy properties depends only on the dispersion of the WNs. The fact that the low-energy property are perfectly compatible with a Weyl fermion picture can also be observed from the optical conductivity shown in Fig. 3b. We can in fact observe a linear trend for \( \omega \to 0 \) as we would expect for a three-dimensional WN.

We then proceed to analyze the dispersion of the bands in proximity to the WNs. We compute the band dispersion along the line connecting two adjacent WNs (\( W \to W \)) and two direction \( y \) and \( z \) perpendicular to it and to each other, with \( y \) belonging to the \( xy \) plane (see Fig. 4). When dealing with pair of nodes in close proximity, we are mainly interested in how far apart they are, given that the further apart, the wider the linear range and the stronger the Weyl character of the node will be. In the case of the only pair of nodes in InMnTi\(_2\) their distance is 0.37 Å\(^{-1}\) which is roughly four times the spacing present in the W2 nodes of TaAs and 10 time that of the W1 ones.

The large distance in a pair makes it so that the linear dispersion of a single node holds for a range of 60 meV, allowing the low-energy properties tied to the Weyl fermion picture to manifest in the material. Another two parameters that can be derived from the dispersion are the Fermi velocity tensor and the tilt...
FIG. 3: (a) Plot of the imaginary part of the dielectric function calculated using the Fermi golden rule. (b) Plot of the real part of the optical conductivity. The high energy part is the result of a calculation on a k-point grid with distance 0.05Å⁻¹ with an hole near the WNs of radius 0.05Å⁻¹. The low energy part has been computed on a more refined grid with distance 0.008Å⁻¹ cropped in a sphere of radius 0.05Å⁻¹ around the WNs. The final results is given by the sum of the cropped and anti-cropped grid while taking into account the weights of the two areas respectively.

vector. The latter can also be used as a way to classify the WN as of type I or II. In the case of InMnTi₂ we observe that its nodes are of type I, given that the tilt of the node is not strong enough.

We then proceeds to compute the surface states of the material, for a tetragonal supercell cut along the [001] direction. The angular resolved photoemission spectroscopy (ARPES) of both the Ti- and In-terminated surfaces are shown in Fig. [3]. A clear distinction between the bulk and surface state can be observed, where the bulk states given the intensity of the plot. In Fig. [3]b we can observe a plot of the Fermi surface, where the projections of the WNs have been highlighted. As we would expect, open lines connecting such projection, commonly known as "Fermi arcs" are present and can be seen connecting pair of nodes within the same or the neighboring cell. We can also compute the spectral function along the direction connecting the projection of two Weyl nodes with opposite chirality Fig. [3]. Here we can observe a surface band leaking from one bulk node into the other which is directly related to the Fermi arcs. The shape of this band is expected to be flat if the arc connecting the 2 nodes follows the shortest path.

Finally we compute the Berry curvature by means of Wannier interpolation on a sphere of points around a Weyl node (Fig. [3]). The plot shows the results as colored arrows, where the color represent the contribution of the Berry curvature vector to the flux on the surface element of the sphere. The integral of the flux will give the Chern number associated with the node. The analysis shows that the two neighboring nodes belonging to a pair are of opposite chirality as we would expect. The results from the study of the evolution of theHWCCs corroborates the previous results, showing that the two nodes are of chirality +1 and -1 respectively.

IV. CONCLUSIONS

In this work we studied the properties of the newly discovered type-I antiferromagnetic Weyl semimetal InMnTi₂. We show that including the Hubbard correction is fundamental in order to obtain the correct magnetic state and Weyl nodes character. We also shows that, thanks to the separation of the nodes within a pair and the lack of trivial points, this material constitute an ideal candidate for possible future experimental studies for applications related to the low-energy Weyl fermion picture. Both these characteristic also reflects on the quality of the observable Fermi arcs which are clearly defined and well separated from the bulk states. Finally, the presence of only one kind of Weyl nodes makes the analysis of the low-energy properties much easier when compared to other well known WSs such as the transition metal monopnictides.

V. ACKNOWLEDGEMENTS

This research was supported by the NCCR MARVEL, a National Centre of Competence in Research, funded by the Swiss National Science Foundation (grant number 182892).

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FIG. 4: Plot of the DFT (dashed blue) and Wannier (red) band dispersion in proximity of a Weyl node. The $W \rightarrow W$ $x$ direction is set to lie that joins a pair of adjacent Weyl nodes. The $y$ and $z$ directions are chosen to be perpendicular to $x$ and each other with $y$ laying in the $xy$ plane.
FIG. 5: Surface states computed with the iterative Green’s function method on top of the wannierization for both the titanium and indium terminated surfaces cut along the [001] direction. (a) ARPES plot along the high-symmetry path in proximity of the fermi level (b) ARPES plot along the $W \rightarrow W$ direction. The touching point of the Weyl nodes from the bulk states is clearly visible, as well as the more pronounced bands related to the Fermi arcs that joins the 2 nodes. (c) Fermi surface of the surface states computed at $\mu = -0.096$. The red (blue) dots represent the projection of the Weyl nodes with chirality $+1(-1)$. The Fermi arcs going from nodes of opposite chirality can be observed.

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FIG. 6: Plot of the Berry curvature on a sphere around 2 neighboring WNs. The color of the arrows shows its respective sign of the contribution for the flux. As expected the two neighboring node exhibit opposite chirality. This can be identified qualitatively by seeing that one node shows a preponderance of positive flux (red arrows), while the other a preponderance of negative flux (blue arrows). The chirality of said nodes as also been confirmed using the HWCCs implemented in Z2pack which corroborates the results from the Wannier interpolation carried out with WannieBerri.

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