Multiple band-crossings and Fermi surface topology: role of double nonsymmorphic symmetries in MnP-type crystal structures

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We use relativistic ab-initio methods combined with model Hamiltonian approaches to analyze the normal-phase electronic and structural properties of the recently discovered WP superconductor. Remarkably, the outcomes of such study can be employed to set fundamental connections among WP and the pressure induced superconductors CrAs and MnP compounds belonging to the same space group. One of the key features of the resulting electronic structure is represented by the occurrence of multiple band crossings along specific high symmetry lines of the Brillouin zone. In particular, we demonstrate that an eight-fold band degeneracy is obtained along the S-R path at \((k_x, k_y) = (\pi, \pi)\), due to time reversal invariance and a pair of nonsymmorphic symmetries. The presence of multiple degenerate Fermi points along the S-R direction constraints the topology of the Fermi surface, which manifests distinctive marks when considering its evolution upon band filling variation. We show that, by changing the relative position of the Fermi level with respect to the eight-fold degenerate bands, one can tune the effective dimensionality of the Fermi surface. If the Fermi level does not cross the multifold degenerate bands, as for the WP and CrAs compounds, the degeneracy forces the occurrence of two-dimensional (2D) Fermi surface sheets centered around the S-R line with a corrugated profile along the \(k_z\) direction. On the contrary, these surfaces are converted into open or closed Fermi pockets, if the bands along the SR line cross the Fermi level, as it happens in MnP. Moreover, we show that the spin-orbit interaction determines a selective removal of the band degeneracy and, consequently, a splitting of the quasi 2D Fermi sheets, as it happens in WP.

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I. INTRODUCTION

Recent years have testified an increasing interest in the study of nodal metals with protected band degeneracies near the Fermi level, especially due to the rapid development of the field of topological condensed matter.129

Topological gapless phases are marked by topologically protected Fermi surface which occur as a consequence of band crossings associated with a topological number that in turn is tied to the symmetries enforcing the band degeneracy. The significant advancements in the classification schemes based on topology and in materials predictions led to the discovery of a wide number of topological semimetals (SMs) that include both Dirac and Weyl SMs22,23 nodal line52,27, type-I and type-II SM25,29, multifold SM29.

It is well known that in crystals degeneracies can also come from non point-group types of symmetries. For instance, nonsymmorphic crystaline symmetries, namely symmetries that involve not only point group operations but also non-primitive lattice translations, typically force bands to cross and can enforce the occurrence of unconventional topological phases.22,23,41,43

Nonsymorphic symmetries when combined with inversion, time or particle-hole symmetry transformations can allow band degeneracies at the origin or at the boundary of the Brillouin zone (BZ).35 Moreover, such nonsymmorphic nodal systems can also exhibit topologically protected Fermi surfaces of reduced dimensionality, as well as topological response phenomena with non-standard magneto-transport properties 33,34.

Among the materials exhibiting nonsymmorphic crystal symmetries, a remarkable case is represented by the CrAs, especially in view of the promising possibility to combine non-standard nodal electronic states with magnetic and superconducting orderings.44,45 CrAs belongs to transition metal pnictides with formula MX (M =transition metal, X =P, As, Sb), having orthorhombic MnP-type crystal structure at ambient conditions.45 A member of the same family is the MnP that shares with the CrAs a superconducting phase driven by external pressure and akin to the magnetism, suggesting a new form of superconductivity with non-conventional order parameter.45

In both compounds the critical temperature-external pressure phase diagram has a typical dome-shaped behaviour 44,45.
with the superconductivity appearing at the critical pressure $P$ equal to 0.7 GPa for CrAs and 8 GPa for MnP, where the helimagnetic transition is suppressed. Another common and salient feature of the phase diagram of these compounds is the presence of tunable magnetic phases that can coexist with superconductivity, exhibit different types of ordered patterns (e.g., helimagnetism, ferromagnetism, metamagnetism, non-standard magnetic anisotropy), or undergo a variety of phase transitions upon cooling, doping, and application of external pressure.

Very recently, Liu et al. found a new superconductor, namely the WP, belonging to this class of transition metal pnictides, with a bulk superconductivity appearing at 0.84 K, at ambient pressure. Remarkably, the WP is the first $5d$ transition metal phosphide with a non magnetic ground state. The extended $5d$-shells lead to a strong coupling between the W $d$-orbitals and the neighboring $p$-orbitals, giving rise to a crystal structure more distorted than that of CrAs and MnP. Moreover, the W-$5d$ electrons exhibit spin-orbit coupling interaction stronger than the $3d$ of the CrAs and MnP.

In this paper, we employ density functional theory (DFT), supported by the formulation of an effective low-energy model Hamiltonian, to investigate the electronic band-structure of WP, comparing it with the non-magnetic phase of the CrAs and MnP. We demonstrate that the presence of nonsymmorphic crystal symmetries, other than time-reversal and inversion symmetries, allows for additional degeneracies in the band spectrum, along some high-symmetry paths of the BZ. In particular, we show that an extra four-fold degeneracy, beyond Kramers degeneracy, is due to the invariance of the Hamiltonian with respect to a pair of nonsymmorphic transformations acting along the SR line of the BZ, and we derive the explicit common basis along the high symmetry lines.

Then, we analyze the symmetry constraints on the topology of the Fermi surface by considering different band fillings. We show that, if there are no Fermi points along the SR line, the degeneracy forces the formation of two-dimensional (2D) Fermi surface sheets centered around the SR line at $(k_x,k_y)=(\pi,\pi)$ with a corrugated profile along the $k_z$ direction. Otherwise, the bands along the SR line cross the Fermi level thus contributing to the formation of eight Fermi surfaces that in turn can get converted into Fermi pockets and stripe-shaped Fermi lines.

The paper is organized as follows: in the next section we describe the computational details of the ab-initio calculations. In section III we compare the structural properties of WP with those of CrAs and MnP, whereas in section IV we present our DFT results for the electronic band structure and related density of states. Section V is devoted to the explicit derivation of the nonsymmorphic symmetry operators and to demonstrate the eight-fold degeneracy along the S-R line, while in section VI we calculate the Fermi surfaces for the different compounds. Finally, the last section is devoted to the final remarks and conclusions.

II. COMPUTATIONAL DETAILS

We have performed DFT calculations by using the VASP package. The core and the valence electrons were treated within the Projector Augmented Wave (PAW) method with a cutoff of 400 eV for the plane wave basis. We have used a PAW with 6 valence electrons for the W ($6s^25d^4$), 7 valence electrons for the Mn ($4s^23d^5$) and 5 valence electrons for the P ($3s^23p^3$). The calculations have been performed using a $12\times16\times10$ k-point Monkhorst-Pack grid for the non polarized case and a $6\times8\times6$ k-point Monkhorst-Pack grid for the case with spin-orbit coupling (SOC). In the first case we have a 240 k-points in the independent BZ, while we have 288 k-points in the case with SOC. For the treatment of exchange-correlation, the generalized gradient approximation (GGA) has been used. For the CrAs, we have used the computational setup of reference.

We have optimized the internal degrees of freedom by minimizing the total energy to be less than $7\times10^{-7}$ eV. After obtaining the Bloch wave functions $\psi_{n,k}$, the Wannier functions $W_n(r)$ have been built up using the WANNIER90 code, generalizing the following formula to get the Wannier functions $W_n(r)$:
\[ W_n(r) = \frac{V}{(2\pi)^3} \int d\mathbf{k} \psi_{n,k} e^{-i\mathbf{k}\cdot\mathbf{r}}, \]

were \( V \) is the volume of the unit cell and \( n \) is the band index.

To extract the low energy properties of the electronic bands, we have used the Slater-Koster interpolation scheme. In particular, we have fitted the electronic bands, in order to get the hopping parameters and the spin-orbit constants. This approach has been applied to determine the real space Hamiltonian matrix elements in the maximally localized Wannier function basis, and to find out the Fermi surface with a 50×50×50 \( k \)-point grid.

### III. STRUCTURAL PROPERTIES

WP belongs to the family of transition-metal pnictides with a general formula MX. Among the various phases exhibited by these compounds, we focus on the orthorhombic MnP-type B31 phase (space group Pnma)\(^\text{[23]}\) being the one where the superconducting phase occurs for WP, CrAs and MnP. The primitive cell contains four M and four X atoms. Each M atom is surrounded by six nearest-neighbour X atoms and it is located at the centre of MX\(_6\) octahedra, which are face-sharing as shown in Fig. 1\(^\text{[24]}\). Four of the six bonds are inequivalent due to the large anisotropy exhibited by this class of compounds. In Table I, we compare the structural properties of WP, CrAs and MnP at ambient pressure with the ideal high-symmetry crystal structure of the WP. The lattice constants are given by: \( a = \sqrt[3]{2} \sqrt{\frac{V}{8}}, b = \sqrt[3]{2} \sqrt{\frac{V}{2}}, c = \sqrt[3]{V} \sqrt{2} \), where \( V \) is the volume of primitive cell of the WP. We point out that the lattice constants, atomic positions and the bond lengths for the CrAs and MnP come from experimental results\(^\text{[68,69,72,81]}\) while those of WP have been calculated in this work by using the atomic relaxations in DFT.

We notice that \( a \) and \( c \) of the WP are larger than those of CrAs and MnP; the \( b \) lattice constant of CrAs is the largest and it is responsible for the antiferromagnetic transition exhibited by this compound.\(^\text{[23]}\) In the Table I, we also report the values of the four inequivalent bonds M-X\(_1\)-M-X\(_4\), and observe that M-X\(_2\) and M-X\(_3\) are almost degenerate. Finally, we have computed the polyhedral volume (PV), namely the volume of the octahedra that can be build around the M atoms, and the bond angle variance (BAV) of these octahedra, which we define as \( \sum_{i=1,6} |\theta_i - \theta_0|^2 \) where \( \theta_0 \) is the ideal bond angle equal to 90° for a regular octahedron. Concerning the PV, we notice that the value for WP is larger than MnP since the atomic radius of W is larger with respect to Mn. Moreover, the PV of CrAs has the largest value because of the large volume of the As. The estimated BAV values show that the WP exhibits a more distorted structure if compared to CrAs and MnP.

|                | WP\(^\text{[24]}\) | CrAs\(^\text{[25]}\) | MnP\(^\text{[45,51]}\) | HSS |
|----------------|-----------------|-----------------|-----------------|-----|
| Bond length(Å) |                 |                 |                 |     |
| M-X\(_1\)      | 2.5342*         | 2.5736          | 2.3938          | 0   |
| M-X\(_2\)      | 2.4967*         | 2.5116          | 2.3848          | 1/4 |
| M-X\(_3\)      | 2.4973*         | 2.4653*         | 2.3848          | 1/4 |
| M-X\(_4\)      | 2.4653*         | 2.5116          | 2.2803          | 1/2 |
| PV(Å\(^3\))    | 19.212*         | 20.565          | 16.367          | 19.212 |
| BAV (deg.\(^2\)) | 191.49*        | 77.708          | 142.98          | 0   |

* present work

### IV. ELECTRONIC PROPERTIES

In this section, we present the DFT based results of the electronic properties of WP. We start by considering the DOS computed for each of the crystal structure discussed in the previous section, in order to extract the dominant orbital character in the different regions of the energy spectrum. Then, we present the electronic band structure using the crystal parameters reported in Table I.

#### A. Density of states and crystal-field energy levels

Here, we investigate the density of states and in particular the evolution of the \( d \) energy levels focusing on the \( 3x^2 - r^2 \) states that are the lowest non-degenerate energy levels in the face-shared octahedral crystal field.\(^\text{[52]}\) We notice that \( x \) is the direction orthogonal to the face-sharing surfaces. This issue is performed by looking at the density of states (DOS) of WP in three cases: firstly, we consider the ideal high-symmetry crystal structure as that quoted in the Table I then, we consider the experimental volume and the ideal high-symmetry atomic positions, and finally, we examine the experimental structure with the atomic positions calculated from the atomic relaxation procedure.

In the first case, the \( 3x^2 - r^2 \) DOS presents the largest peak at about 5 eV below the Fermi level as we can see from the Fig. 2. In the second case, there is a mixing be-
between different energy levels, producing two large peaks approximately located at -4 eV and +2 eV, as it can be observed by inspection of Fig. 3. In the third case, corresponding to the fully distorted structure, the Fig. 4 shows that the peak of the $3x^2 - r^2$ DOS is set at about 3 eV above the Fermi level. Thus, moving from the ideal structure to the fully distorted structure, the $3x^2 - r^2$ energy level peaks move from occupied to unoccupied configurations. One of the reason why the energy levels change so drastically as a function of the structural properties in this family is the weakness of the crystal field. Indeed, in strongly ionic systems, like in transition metal oxides, the transition metal atom is surrounded by atoms with filled p-shells, producing a weaker crystal field. Moreover, the strongly distorted structure, favored by the weak crystal field, produces a mixing of the orbital character of the d-bands making impossible to identify a subset of d-orbital close to the Fermi level.

Referring to the character of the bands, we infer that the bands close to the Fermi level are primarily due to the W degrees of freedom, so they are more flat with respect to the bands that are located 4 eV above and below the Fermi level, and lead to the van Hove singularities. The latter bands may assigned to P states, and are more delocalized with respect to the W ones.

In all three cases considered, the character of the DOS from -8.5 eV to -6 eV is predominantly P-3p, while from -6 eV to 4 eV the W-5d states dominate, and finally, above 4 eV there is a mixing between P-3p, P-4s and W-6s states. We remark that, since the W bands are due to 5d orbitals, the bandwidth is much wider than that of CrAs and MnP, so that we may suppose that the WP is the least correlated system between the three transition metal pnictides investigated. As for CrAs, it is hopeless to entirely decouple the W-5d states close to the Fermi level from the P-3p states in an accurate way, because of the strong hybridization between them, as we show in the Appendix. Nevertheless, an accurate effective model for a reduced number of d-bands can be obtained also in the present case of strong hybridization as we show in the Appendix.

B. Band structure and effect of the spin-orbit coupling on the band degeneracy

In order to set the electron filling, first of all, one has to recall that the oxidation state of WP is predominantly...
In Figs. 5-6 we show the band spectrum derived from first principle calculations, in the cases where the spin orbit coupling is included or not in the calculations. The bandwidth is around 16 eV and, as already pointed out for the DOS, there are flat bands near the Fermi level, due to the W degrees of freedom, while the wider bands located far from the Fermi level are mainly due to the phosphorus atoms.

Figure 5. Band structure of the WP along the high-symmetry path of the orthorhombic BZ without (green lines) and with SOC (red lines). We plot in the energy range from -9 eV to +9 eV (top panel) and from -2 eV to +2 eV (bottom panel). The Fermi level is set at the zero energy.

Figure 6. Band structure of the WP along the remaining high-symmetry lines of the orthorhombic BZ without (green lines) and with SOC (red lines). We plot in the energy range from -9 eV to +9 eV (top panel) and from -2 eV to +2 eV (bottom panel). The Fermi level is set at the zero energy.

0, while in MnP the oxidation state is +1 for the Mn and -1 for the P. Indeed, if the oxidation state of Mn had been zero, then Mn would have been in 3d$^7$ configuration with a maximum magnetic moment of 3 $\mu_B$. However, with GGA+U calculations and at high volumes, we can see that the magnetization exceeds 3 $\mu_B$ per Mn atom. Therefore, the Mn oxidation state is not zero, but it is +1 in MnP compound, implying that the oxidation state of the phosphorus ions is -1 in the MnP. This suggests that also the oxidation state of the Cr can be +1 in CrP. We also stress that the oxidation state of CrAs is zero, similarly to WP one.

The relevant features of the band structure without SOC may be ascribed to the symmetries of the underlined Hamiltonian that may describe the system. Since the system is symmetric under the unitary inversion operator $\hat{P}$ and upon the action of the time-reversal operator $\hat{T}$, the antiunitary inversion-time reversal operator $\hat{P}\hat{T}$ operator gives rise to bands that are two-fold degenerate at any k-vector of the BZ. This is the Kramers degeneracy and it is protected under the action of SOC. The system possess also nonsymmorphic symmetries, which involve half translation of a Bravais lattice, causing an additional degeneracy along specific lines of the BZ. This additional degeneracy, which can be two-fold in case of one nonsymmorphic symmetry or four-fold in case of two nonsymmorphic symmetries, is active only along some high-symmetry lines because the corresponding operators are momentum-dependent. In particular, along the SR line the band structure carries an overall eight-fold degeneracy due to the presence of two nonsymmorphic symmetries. Such multifold degeneracy is also expected to
effectively reduce the probability for the bands to cross the Fermi level and thus they can induce some consequences on the dimensionality of the Fermi surface, as we will consider in more details in the next sections.

The interplay between the SOC interaction and the inter-orbital degrees of freedom allows for a selective removal along some lines of the BZ of the band degeneracy ascribed to the crystal symmetries. Specifically, the SOC partially removes the degeneracy of the bands along the XS, TZ, YT and SR high-symmetry lines, bringing them from four-fold to two-fold degeneracy along the first three and from eight-fold to two-fold degeneracy along the last one, as we show in the Figures of the BZ reported in the Appendix. Instead, at the point R and S, the SOC partially removes the degeneracy bringing it from eight- to four-fold. The splitting due to the SOC along the SR line is relatively small and it does not change the dimensionality of the Fermi surface. We would like to point out that the spin-orbit coupling constants $\lambda$ estimated from the real space Hamiltonian for the W and P atoms are $\lambda_W=-228\text{ meV}$ for the $5d$-orbitals of the W atoms and $\lambda_P=55\text{ meV}$ for the $3p$-orbitals of the P atoms, respectively. As a consequence the SOC splitting strongly affects the bands near the Fermi level because these bands mainly have a W character, and this effect turns out to be relevant for the transport properties. Although the SOC splitting is larger in WP compound than in CrAs and MnP systems,$^{53}$ the selective removal of the band degeneracy due to the crystal symmetries is also present in these latter materials.

Due to the eight-fold degeneracy and the presence of the two nonsymmorphic symmetries, each minimal model should contain at least four bands, which are equivalent to two bands per formula unit. As a consequence, the system will be always metallic if the time reversal symmetry breaking, the protection of the degeneracy due to the crystal symmetries is also present in these latter materials.

Because of the symmetries of the system, we will have semi-Dirac-like energy-momentum dispersions near the points X, Y and Z of the BZ. In particular, as already mentioned above, the semi-Dirac point at Y has been proposed to produce the linear magnetoresistance in CrAs and MnP.$^{54,55}$ The band structure in Figs. 3, 4 shows a semi-Dirac point at 0.02 eV below the Fermi level suggesting that linear dependent magnetoresistance could be also found in the WP compound. In the case of time reversal symmetry breaking, the protection of the degeneracy can be partially removed depending on the magnetic order. Thus, if we consider an antiferromagnetic order along the x-axis, a ferromagnetic order along the y-axis and an antiferromagnetic order along the z-axis the degeneracy is reduced along XS and SR symmetry lines.$^{56}$

We conclude this section noticing that the results here presented for the band spectrum and DOS share robust qualitative features with those of the CrAs$^{51}$ and MnP compounds.$^{53}$

V. NONSYMMORPHIC SYMMETRIES ALONG THE SR LINE

In this section we demonstrate that the presence of nonsymmorphic symmetries brings to additional degeneracies along specific lines of the BZ in the case of vanishing SOC interaction, and is at the origin of the eight-fold degeneracy along the SR path the BZ. We start by considering a tight-binding description of the WP electronic structure, whose matrix elements have been set according to the outcome of the DFT calculations. In particular, we restrict to the representative subspace of two $d$-orbitals (i.e. $d_{xy}$ and $d_{yz}$) and consider only non-vanishing projected W-W hopping amplitudes. When the spin degeneracy is considered, one can reduce the analysis by considering separately each spin channel, thus remaining to the outcome of the DFT calculations. In particular, we denote by $t_{\alpha\beta}$, $t_{\alpha\alpha}$ the hopping amplitudes between the sites $\alpha_i$ and $\alpha_j$ (where $i, j = A, B, C, D$ as labelled in Fig. 1) along the direction $\mathbf{ix} + \mathbf{my} + \mathbf{nz}$. The Hamiltonian for each spin-channel is then written as follows:

$$H(k_x, k_y, k_z) = \begin{pmatrix} H_{\alpha\alpha}(k_x, k_y, k_z) & H_{\alpha\beta}(k_x, k_y, k_z) \\ H_{\beta\alpha}(k_x, k_y, k_z) & H_{\beta\beta}(k_x, k_y, k_z) \end{pmatrix},$$

where $\alpha$ and $\beta$ label the $d_{xy}$ and the $d_{yz}$ orbital, and $H_{\beta\alpha}$ is the conjugate transpose of $H_{\alpha\beta}$. The diagonal term of the matrix $H_{\alpha\alpha}$ is expressed as:

$$H_{\alpha\alpha}(k_x, k_y, k_z) = t_1(k_x, k_y, k_z)s_0 \otimes \tau_0 + t_2(k_x, k_y, k_z)s_0 \otimes \tau_x + t_3(k_x, k_y, k_z)s_y \otimes \tau_0 + t_4(k_x, k_y, k_z)s_y \otimes \tau_z + t_5(k_x, k_y, k_z)s_z \otimes \tau_0 + t_6(k_x, k_y, k_z)s_z \otimes \tau_z + t_7(k_x, k_y, k_z)s_0 \otimes \tau_y,$$

where $s_i, \tau_i, \sigma_i$ represent the Pauli matrices for $i = x, y, z$, and the unit matrices for $i = 0$. $s_i$ act in the subspace of spins, $\tau_i$ in the subspace of orbitals, $\sigma_i$ and $\gamma_i$ in the subspace set by the atomic states in the unit cell. An analogous expression to Eq. (3) defines also $H_{\beta\beta}$. The hopping parameters have the following expressions:
The off-diagonal term $H_{\alpha\beta}$ is written as:

$$
H_{\alpha\beta}(k_x) = \begin{pmatrix}
0 & 100 \\
100 & 0 & 0 \\
0 & 0 & 0 \\
100 & 0 & 0 & 0
\end{pmatrix} +
$$

where $t_{100}^{AB\beta\alpha} \neq t_{100}^{AB\alpha\beta}$. Note that all the hoppings are written in units of $a$, $b$ and $c$.

We will now focus on the tight-binding Hamiltonian along the SR line $H_{\alpha\beta}$, where we keep fixed $(k_x, k_y) = (\pi, \pi)$. We notice that, along that high symmetry line, the $t_2(k_x), ..., t_7(k_x)$ hybridization terms in the intra-orbital subspace do vanish. This circumstance reduces $H_{\alpha\beta}$ in a non block-diagonal form, where only the intra-orbital sectors $H_{\alpha\alpha}(k_z)$ and $H_{\beta\beta}(k_z)$ are diagonal.

When we take both spin-channels, we can then consider the two unitary operators:

$$
\begin{align*}
\hat{Q} & = s_0 \otimes \tau_0 \otimes \sigma_y \otimes \gamma_y \\
\hat{U}(k_z) & = \begin{pmatrix} 0 & 1 \\ e^{ik_x} & 0 \end{pmatrix} \otimes \tau_0 \otimes \sigma_z \otimes \gamma_y,
\end{align*}
$$

where $\gamma_i$ represent the Pauli matrices for $i = x, y, z$, and the unit matrices for $i = 0$. The operators $\hat{Q}$ and $\hat{U}(k_z)$ commute with the Hamiltonian $H_{\alpha\beta}(k_z)$ along the S-R path:

$$
\begin{align*}
[H, \hat{Q}] & = 0, \quad \text{at } (k_x, k_y) = (\pi, \pi) \\
[H, \hat{U}(k_z)] & = 0, \quad \text{at } (k_x, k_y) = (\pi, \pi).
\end{align*}
$$

Moreover, they anticommute with each other:

$$
\{ \hat{Q}, \hat{U}(k_z) \} = 0.
$$

In particular, $\hat{Q}$ acts by exchanging the coordinates of A and D atoms within the unit cell; $\hat{U}(k_z)$ is instead
a nonsymmmorphic operator involving half translation of
the reciprocal lattice and a transformation on the unit
cell configurations, which satisfies the following relation:

$$\hat{U}^2(k_z) = e^{i k_z} I,$$  \hspace{1cm} (11)

whose eigenvalues are $\pm e^{i k_z/2}$, and where $I$ is the identity matrix.

Along the SR line, $H(k_z)$ also commutes with other two
unitary operators:

$$\hat{V} = s_0 \otimes \tau_0 \otimes \sigma_z \otimes \gamma_y \hspace{1cm} (12)$$

$$\hat{W}(k_z) = \begin{pmatrix} 0 & e^{i k_z} & 1 \end{pmatrix} \otimes \tau_0 \otimes \sigma_y \otimes \gamma_y \hspace{1cm} (13)$$

$$\left[ \hat{H}, \hat{V} \right] = 0, \hspace{0.5cm} \text{at} \hspace{0.5cm} (k_x, k_y) = (\pi, \pi) \hspace{1cm} (14)$$

$$\left[ \hat{H}, \hat{W}(k_z) \right] = 0, \hspace{0.5cm} \text{at} \hspace{0.5cm} (k_x, k_y) = (\pi, \pi) \hspace{1cm} (15)$$

Moreover, $\hat{V}$ and $\hat{W}(k_z)$ anticommute with each other:

$$\{ \hat{V}, \hat{W}(k_z) \} = 0, \hspace{1cm} (16)$$

We notice that $\hat{V}$ acts by exchanging the coordinates of
B and C atoms within the unit cell, while $\hat{W}(k_z)$, apart
from acting on the intra-unit cell orbital degrees of free-
dom, is a nonsymmmorphic operator involving half trans-
lation of the reciprocal lattice.

Furthermore, we have that the operators $\hat{Q}, \hat{V}, \hat{W}(k_z)$ and
$\hat{U}(k_z)$ fulfill the following algebra:

$$\{ \hat{Q}, \hat{V} \} = 0,$$ \hspace{1cm} (17)

$$\left[ \hat{Q}, \hat{W}(k_z) \right] = 0 . \hspace{1cm} (18)$$

$$\left[ \hat{U}(k_z), \hat{V} \right] = 0,$$ \hspace{1cm} (19)

$$\left[ \hat{U}(k_z), \hat{W}(k_z) \right] = 0,$$ \hspace{1cm} (20)

Since $\hat{U}$ and $\hat{V}$ commute between each other and with
the Hamiltonian, it is possible to choose a common eigenstate
$\psi_{uv}$, labeled by the corresponding $u$ and $v$ eigenvalues of
$\hat{U}$ and $\hat{V}$, associated to the same energy $E(k_z)$:

$$\hat{U}\psi_{uv} = u\psi_{uv}, \hspace{0.5cm} \hat{V}\psi_{uv} = v\psi_{uv} . \hspace{1cm} (21)$$

$$H(k_z)\psi_{uv} = E(k_z)\psi_{uv} \hspace{1cm} (22)$$

Then, by using the commutation and anticommutation relations between the above operators (see the Eqs. (10),
(16) and (17) – (20)), one can have:

$$\hat{U}(\hat{Q}\psi_{uv}) = -u(\hat{Q}\psi_{uv}) \hspace{0.5cm} \hat{V}(\hat{Q}\psi_{uv}) = -v(\hat{Q}\psi_{uv}), \hspace{1cm} (23)$$

$$\hat{U}(\hat{W}\psi_{uv}) = u(\hat{W}\psi_{uv}) \hspace{0.5cm} \hat{V}(\hat{W}\psi_{uv}) = -v(\hat{W}\psi_{uv}), \hspace{1cm} (24)$$

$$\hat{U}(\hat{Q}\hat{W}\psi_{uv}) = -u(\hat{Q}\hat{W}\psi_{uv}) \hspace{0.5cm} \hat{V}(\hat{Q}\hat{W}\psi_{uv}) = v(\hat{Q}\hat{W}\psi_{uv}), \hspace{1cm} (25)$$

Eqs. (21) – (25) show that it is possible to construct a
subspace associated to the same energy eigenvalue, spanned by the four orthogonal basis states: $\psi_{uv}$, $\hat{Q}\psi_{uv}$, $\hat{W}\psi_{uv}$ and $\hat{Q}\hat{W}\psi_{uv}$. The dimensionality of this subspace
equals the four-fold degeneracy which is obtained along the SR line, for each of the spin channels. We finally
point out that the inclusion of the SOC interaction in the
tight-binding Hamiltonian partially removes the degener-
cacy, bringing it from eight-fold to two-fold. This is be-
cause the total Hamiltonian is no longer invariant upon $\hat{Q}$, $\hat{U}$, $\hat{V}$ and $\hat{W}$. On the contrary, the SOC interaction
does not remove the Kramers degeneracy associated to the
combination of inversion and time reversal symmetry.

The results of the presented analysis allow us to conclude
that the four-fold degeneracy for each spin channel is due
to the existence of two couples of anticommuting symme-
try operators, two of them being nonsymmmorphic, which
satisfy the algebra given by Eqs. (10), (16) and (17) –
(20).

VI. EFFECT OF THE NONSYMMORPHIC
SYMMETRIES ON THE FERMI SURFACE

In this section we investigate the evolution of the Fermi
surfaces (FS) as a function of the electron filling. We will
start by considering the case of vanishing SOC, while at
the end of this section the effects of the SOC term will
be discussed.

The FS of the WP are deduced at ambient pressure
whereas those of the CrAs and MnP are derived at the
critical pressures where the magnetism is suppressed and
the superconductivity comes in. In the case of CrAs, we
use the results from the literature. Instead, for the MnP the experimentally measured pressure ampli-
date that suppresses the magnetism is 7 GPa, while
from our ab-initio calculations we find that the magneti-
zation goes to zero with a metamagnetic transition when

$$\hat{U}\psi_{uv} = u\psi_{uv}, \hspace{0.5cm} \hat{V}\psi_{uv} = v\psi_{uv} . \hspace{1cm} (21)$$

$$H(k_z)\psi_{uv} = E(k_z)\psi_{uv} \hspace{1cm} (22)$$

Then, by using the commutation and anticommutation relations between the above operators (see the Eqs. (10),
(16) and (17) – (20)), one can have:

$$\hat{U}(\hat{Q}\psi_{uv}) = -u(\hat{Q}\psi_{uv}) \hspace{0.5cm} \hat{V}(\hat{Q}\psi_{uv}) = -v(\hat{Q}\psi_{uv}), \hspace{1cm} (23)$$

$$\hat{U}(\hat{W}\psi_{uv}) = u(\hat{W}\psi_{uv}) \hspace{0.5cm} \hat{V}(\hat{W}\psi_{uv}) = -v(\hat{W}\psi_{uv}), \hspace{1cm} (24)$$

$$\hat{U}(\hat{Q}\hat{W}\psi_{uv}) = -u(\hat{Q}\hat{W}\psi_{uv}) \hspace{0.5cm} \hat{V}(\hat{Q}\hat{W}\psi_{uv}) = v(\hat{Q}\hat{W}\psi_{uv}), \hspace{1cm} (25)$$

Eqs. (21) – (25) show that it is possible to construct a
subspace associated to the same energy eigenvalue, spanned by the four orthogonal basis states: $\psi_{uv}$, $\hat{Q}\psi_{uv}$, $\hat{W}\psi_{uv}$ and $\hat{Q}\hat{W}\psi_{uv}$. The dimensionality of this subspace
equals the four-fold degeneracy which is obtained along the SR line, for each of the spin channels. We finally
point out that the inclusion of the SOC interaction in the
tight-binding Hamiltonian partially removes the degener-
cacy, bringing it from eight-fold to two-fold. This is be-
cause the total Hamiltonian is no longer invariant upon $\hat{Q}$, $\hat{U}$, $\hat{V}$ and $\hat{W}$. On the contrary, the SOC interaction
does not remove the Kramers degeneracy associated to the
combination of inversion and time reversal symmetry.

The results of the presented analysis allow us to conclude
that the four-fold degeneracy for each spin channel is due
to the existence of two couples of anticommuting symme-
try operators, two of them being nonsymmmorphic, which
satisfy the algebra given by Eqs. (10), (16) and (17) –
(20).

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use the results from the literature. Instead, for the MnP the experimentally measured pressure ampli-
date that suppresses the magnetism is 7 GPa, while
from our ab-initio calculations we find that the magneti-
zation goes to zero with a metamagnetic transition when
the volume is uniformly reduced by 5.8%. Therefore, we apply the theoretically predicted volume, which is reduced of 5.8% with respect to the ambient pressure, for proceeding further about the determination of the Fermi surface. For completeness, we mention that the metamagnetic transition can be accounted by considering the van Hove singularities close to Fermi level.\[65,66\]

We start with some general considerations and first consider the case of Fermi points along the SR line. If the bands along the SR direction cross the Fermi level, we have eight Fermi points \((\pm \pi, \pm \pi, \pm k_F)\) due to the inversion and mirror symmetry in this class of compounds. The Fermi points \((\pm \pi, \pm \pi, \pm k_F)\) are eight-fold degenerate, four-fold because of the intracell orbital degrees of freedom, which are connected by two nonsymmorphic symmetries, and two-fold because of the time reversal symmetry. Since the electronic structure along the SR line does not have a semimetallic behavior, due to the Kramers degeneracy in the whole BZ, in any plane that includes the SR line there are four Fermi lines emerging from the Fermi points which can evolve in various ways by ending into the other Fermi points. Many possible combinations are possible, however, an even number of Fermi points should be connected because of inversion and mirror symmetries.

As example of this class of compounds, we examine the case of the MnP. We show \((k_y,k_z)\) side view of the FS cartoon since it is the only one interesting in this case. In Fig. 7, the three connections that we observed in the MnP compound are depicted. These Fermi surfaces can connect two points inside the first BZ forming a pocket \((C_1)\), four points forming a stripe \((C_2)\) and two points belonging to the first and second BZ forming a pocket \((C_3)\).

![Figure 7. (k_y,k_z) plane side view of the connections obtained in the MnP compound. The Fermi points at \((\pm \pi, \pm \pi, \pm k_F)\) are represented by the open circles.](image)

At this stage it is useful follow the band structure of the MnP along the path S-X-T-R-S and investigate the evolution of the Fermi surfaces as function of the filling of the system \(n\). As we show in Fig. 8, we define \(n_1\) and \(n_3\) as the filling at which the Fermi level crosses the bands at the S point and R point, respectively, while \(n_2\) is the filling at which the Fermi level touches the extreme points along the SX and TR lines. The filling \(n_1\), \(n_2\) and \(n_3\) very roughly define regions where we can observe different Fermi surfaces scenarios.

When \(n\) is slightly larger than \(n_1\), we have some Fermi pockets close to the S point but we do not have Fermi points along the RS line. When \(n=n_1\) we have an eight-fold Fermi point at S. When \(n_2 \leq n < n_1\) we have four connections of the kind \(C_1\). Two connections are shown in Fig. 9(a) and two are shown in Fig. 9(b). When \(n_2 < n < n_1\) we have two connections of the kind \(C_1\) in Figs 10(a) and two connection of the kind \(C_2\) in Fig. 10(b). When \(n_3 < n < n_2\) we have two connections of the kind \(C_1\) in Figs 11(a) and two connections of the kind \(C_3\) in Fig. 11(b). In summary, two connections are always of the kind \(C_1\), while the other two evolve from \(C_1\) to \(C_2\) and finally to \(C_3\).

When \(n=n_3\) the Fermi points reach the R point. Reducing \(n\) and considering that the Fermi surfaces of the kind \(C_1\) cannot disappear, the Fermi points can only move along \(k_y\) forming the 2D Fermi surfaces. This implies that there will be open Fermi surfaces almost parallel to \(k_z\). Finally, when \(n<n_2\) the two Fermi pockets of the kind \(C_1\) evolve in two 2D-Fermi surfaces, while the two Fermi pockets of the kind \(C_3\) disappear. We thus obtain the 2D FS, as we show in Fig. 12(a) and 12(b).

We now proceed with the explicit comparison of the Fermi surfaces (FS) of the normal phase of the CrAs,

![Figure 8. Band structure of MnP along the S-X-T-R-S high-symmetry lines of the orthorhombic BZ without SOC. We plot in the energy range from -0.8 eV to +0.8 eV. The unmodified Fermi level is set at the zero energy.](image)
Figure 9. Fermi surface of MnP in the first BZ without SOC with filling $n_2 < n < n_1$. In panel a) we show two Fermi surfaces emerging from the Fermi points along the RS line, while in panel b) all the other Fermi surfaces. For a better visualization we plot one FS in the BZ and another in the reciprocal unit cell.

Figure 10. Fermi surface of MnP in the first BZ without SOC with filling $n_2 < n < n_1$. In panel a) we show two Fermi surfaces emerging from the Fermi points along the RS line, while in panel b) all the other Fermi surfaces. For a better visualization we plot one FS in the BZ and another in the reciprocal unit cell.

MnP and WP compounds. We point out that those materials are characterized by different fillings, which fall into the distinct regimes above considered. The number of pnictide-$p$ and metal-$d$ bands is 16 per formula unit. For CrAs and WP there are 9 electrons per formula unit, while in the case of MnP we have 10 electrons per formula unit. In the case of CrAs and WP, the bands along the SR line do not cross the Fermi level forming two-dimensional Fermi surface sheets centered around the SR high-symmetry line, namely at $(k_x, k_y) = (\pi, \pi)$, and propagating along the $k_z$ direction.

Let us discuss the 2D and 3D features of the FS of the WP plotted in Fig. 13(a) and 13(b). The FS displays a three-dimensional surface around the $\Gamma$ point and two holelike 2D hourglass shaped sheets centred around the SR high-symmetry line, namely at $(k_x, k_y) = (\pi, \pi)$, and in the $ab$ plane. We have to point out that the bands along the SR line are eight-fold degenerate, but when we move along the XS and the SY they splits in two four-fold bands. One of this four-fold bands crosses the Fermi level, as we can see from the the bands along the XS and SY lines plotted in Fig. 15.

This produces the two 2D surfaces that are doubly degenerate due to the inversion-time reversal symmetry and are constrained by the crystal symmetry to be connected along the lines where the degeneracy is four-fold. We emphasise that in this class of compounds a single nonsymmorphic symmetry is not enough to create a Fermi surface with reduced dimensionality, but we need two nonsymmorphic symmetries as above claimed. Since the two nonsymmorphic symmetries are present also in the non-magnetic phase of CrAs and MnP, it is likely to find two 2D Fermi surface sheets propagating along the $k_z$ direction and centred around the SR line. Indeed, from Fig. 14(a) and 14(b), we see that also the CrAs shows a three-dimensional surface around the $\Gamma$ point and two 2D FS. Even in this case, there are two holelike 2D surfaces in the $ab$ plane centred around the SR line, but the FS are more cylindrical than those found in the WP. However, in the magnetic phase, the 2D surfaces around the SR line disappear but other 2D FS appear along other high-symmetry lines of the BZ where one a single nonsymmorphic symmetry takes place.

Finally, we investigate the effect of the SOC on the Fermi surfaces of the WP as representative case of this class. Though the SOC is too small to change the dimensionality of the Fermi surface, it produces selective splittings in the points where the FS is degenerate. We report
Figure 13. Fermi surface of WP at ambient pressure in the first BZ without SOC. In panel a) we show the 2D sheets, while in panel b) the three-dimensional surface around the $\Gamma$ point. Since the two 2D FS are concentric, for a better visualization we plot one FS in the BZ and another in the reciprocal unit cell.

Figure 14. Fermi surface of CrAs at $P=0.94$ GPa in the first BZ without SOC. In panel a) we show the 2D sheets, while in panel b) the three-dimensional surface around the $\Gamma$ point. Since the two 2D FS are concentric, for a better visualization we plot one FS in the BZ and another in the reciprocal unit cell.

Figure 15. Top view of the 2D Fermi surface of WP centred at S point. In panel a) we report the result without SOC while in panel b) the result under the action of SOC. The arrows indicate the points of the Fermi surface four-fold degenerate, where the surfaces are forced by the crystal symmetry to be connected.

VII. CONCLUSIONS

By combining density functional theory with an effective low-energy model Hamiltonian, we have studied the electronic and structural properties of the WP compound in the presence of spin-orbit coupling. The emerging electronic properties are representative of the MnP-type family and also share common features with other members as CrAs and MnP materials. In all these pnictides the $d$-states dominate at the Fermi level while the $p$-states are located both above and below the Fermi level. The highly distorted structure, favored by a weak crystal field potential, produces a strong orbital mixing of the $d$-bands making quite difficult the identification of a reduced subset of $d$-orbitals for an effective model for the low energy description.

The band structure, other than the time-reversal and inversion symmetries, exhibits nonsymmorphic symmetries that bring to four- or eight-fold degeneracy of the bands along some high-symmetry lines of the BZ. Remarkably, nonsymmorphic symmetries have strong implications on the multiplicity and dimensionality of the Fermi surface. Moreover, the evolution of the Fermi surface topology is linked to the presence or not of Fermi points along some high symmetry directions. If the Fermi level crosses the bands along the SR line, there are eight Fermi surfaces with the presence of Fermi pockets and stripes. Depending on the electron filling, the size of Fermi pockets can increase until creating open Fermi surfaces. This picture brings towards multiple concentric 2D-Fermi surfaces in this class of materials. When the role of the SOC is considered, we show that the interplay between the SOC interaction and the inter-orbital degrees of freedom allows a selective removal of the band degeneracy. We point out that 2D Fermi surfaces were observed also in quasi 2D-supercconductors like cuprates, ruthenates, and iron-pnictides. However, while in the iron-pnictides the FS are electron-like, in this class of compounds they are hole-like. Furthermore, the transition-metal pnictides MX are intrinsically 3D while cuprates, iron-pnictides and ruthenates may be considered such as quasi 2D systems. Moreover, the presence of these 2D sheets could affect the transport and superconducting properties of this class of materials. We would like also to stress that the study...
Figure 16. Band structure of three flat $d$-bands and two wide $p$-bands when the $d$-$p$ hybridization is turned off. The Fermi level is set at zero energy.

of nodal excitations could also be relevant when the phonons effects are concerned, allowing to explain the unusual resistivity behavior and possibly shedding light on the mechanism beyond the superconducting pairing.

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VIII. APPENDIX

A. $p$-$d$ hybridization in transition metal pnictides

Here we examine a $p$-$d$ toy model, in order to demonstrate that it is not possible to reduce to a simple minimal model for the entire subset of $d$-bands close to the Fermi level. We start by considering three $d$ and two $p$ bands, where the $p$-bands have a large dispersion, while the $d$-bands are flat in the region between -0.1 and 0.1 eV. In Fig. 16 we show the case in which the hybridization between the $d$- and $p$-orbitals is turned off, while in Fig. 17 we plot the band structure when the hybridization is switched on. From an inspection to these figures, we conclude that one can distinguish the different contribution of the orbitals to the bands in the first case, whereas the same bands are strongly entangled when the $d$-$p$ hybridization is switched on.

This simple example shows that we cannot obtain an accurate minimal model for all three $d$-bands. When the $p$-$d$ hybridization is larger than the difference between the on-site energies of the $p$- and $d$-states, the $d$- and $p$-manifolds cannot be disentangled.

However, an effective minimal model can be achieved by limiting to the single $d$-band crossing the Fermi level, as we can see in Fig. 17. The possibility describe the band structure close to the Fermi level in terms of a minimal set of bands having mainly $d$ character has been recently demonstrated in other transition metal pnictides. We also point out that, when magnetic properties are concerned, the strong hybridizations requires the $p$-channel to be included, like in the Anderson model, thus allowing for a correct interpretation of the magnetism for this class of compounds.

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