Realistic multiband \( k.p \) approach from \textit{ab initio} and spin-orbit coupling effects of InAs and InP in wurtzite phase

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Semiconductor nanowires based on non-nitride III-V compounds can be synthesized under certain growth conditions to favor the appearance of wurtzite crystal phase. Despite the reports in literature of \textit{ab initio} band structures for these wurtzite compounds, we still lack effective multiband models and parameter sets that can be simply used to investigate physical properties of such systems, for instance, under quantum confinement effects. In order to address this deficiency, in this study we calculate the \textit{ab initio} band structure of bulk InAs and InP in wurtzite phase and develop an 8×8 \( k.p \) Hamiltonian to describe the energy bands around \( \Gamma \) point. We show that our \( k.p \) model is robust and can be fitted to describe the important features of the \textit{ab initio} band structure. The correct description of the spin splitting effects that arise due to the lack of inversion symmetry in wurtzite crystals, is obtained with the \( k \)-dependent spin-orbit term in the Hamiltonian, often neglected in the literature. All the energy bands display a Rashba-like spin texture for the in-plane spin expectation value. We also provide the density of states and the carrier density as functions of the Fermi energy. Alternatively, we show an analytical description of the conduction band, valid close to \( \Gamma \) point. The same fitting procedure is applied to the 6×6 valence band Hamiltonian. However, we find that the most reliable approach is the 8×8 \( k.p \) Hamiltonian for both compounds. The \( k.p \) Hamiltonians and parameter sets that we develop in this paper provide a reliable theoretical framework that can be easily applied to investigate electronic, transport, optical, and spin properties of InAs- and InP-based nanostructures.

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I. INTRODUCTION

In the past decade, the development of low dimensional III-V semiconductor nanostructures has witnessed great advances.\textsuperscript{1} For instance, one interesting feature that was observed in the synthesis of III-V nanowires is the appearance of wurtzite (WZ) crystal phase, instead of the usual zinc-blende (ZB).\textsuperscript{2} This created new possibilities of III-V compounds with WZ structure besides the well established nitride based materials. Moreover, controlling the growth conditions, e. g., temperature and III/V ratio, it is possible to achieve not only single crystal phase nanowires\textsuperscript{3–5} but also to mix ZB and WZ regions with sharp interfaces in the same nanostructure, which is known as polytypism.\textsuperscript{6,7} It has been demonstrated that mixed phases greatly affect the physical properties, for example, of the light polarization\textsuperscript{8–10} electron transport,\textsuperscript{11,12} and photocconductivity.\textsuperscript{13}

Among these new III-V compounds with WZ structure, InAs and InP are particularly important. InAs WZ has a large spin-orbit coupling (SOC) which favors the study of spin related phenomena, for instance, spin field-effect transistors,\textsuperscript{14} and the search for the elusive Majorana fermions.\textsuperscript{15} Also, InAs WZ shows remarkable piezoelectric and piezoresistive properties\textsuperscript{16} that, combined with the InAs narrow band gap, can operate in the near-infrared regime. On the other hand, InP is a promising candidate for photovoltaic applications\textsuperscript{17} and for enhancing the efficiency of solar cells.\textsuperscript{18} In fact, a silicon-integrated nanolaser of InP nanowire has already been demonstrated at room temperature with a wide wavelength range due to the WZ/ZB polytypism.\textsuperscript{19} Furthermore, it is also possible to combine InAs and InP WZ compounds in axial\textsuperscript{20} and radia\textsuperscript{21} heterostructures, which opens the path for novel opportunities in band gap engineering.

Theoretically, studies based on WZ III-V compounds including InAs and InP were reported using different \textit{ab initio} approaches. The main focus of these studies was the determination of the lattice parameters, band gaps and SOC energy splittings in the valence band.\textsuperscript{22–27} Of these references, De and Pryor\textsuperscript{22} provide useful information that can be used in effective models, such as the effective masses and the spin splitting parameters. The issue of using these parameters is that they are only valid in the immediate vicinity of the \( \Gamma \) point (\( \sim 2\% \) of the FBZ), limiting the range of physical phenomena that can be investigated. In order to achieve a better description further away from the \( \Gamma \) point, a multiband effective model is desirable. Although \( k.p \) models and parameters are well established for WZ III-nitride compounds,\textsuperscript{28,29} there are only few reports in the literature for non-nitrides, such as InP\textsuperscript{30,31} and GaAs.\textsuperscript{32}

In this study, we develop a robust 8×8 \( k.p \) Hamiltonian to describe the \textit{ab initio} band structure calculated by WIEN2k\textsuperscript{32} of InAs and InP in WZ phase. We show that our fitted parameters reproduce the \textit{ab initio} band structure, capturing the important anti-crossings.
and spin splitting features up to 1.0 nm$^{-1}$ ($\sim 10\%$ of the FBZ in the $k_xk_y$ plane and $\sim 22\%$ in the $k_z$ direction). At $\Gamma$ point, each band is two-fold degenerate and for the valence band we found that the band ordering, from top to bottom, is HH (heavy hole), CH (crystal field split-off hole) and LH (light hole) for InAs and HH, LH and CH for InP. This ordering is due to an interplay of SOC energy splittings and the crystal field energy splitting. The intricate behavior of spin splittings, arising from the bulk inversion asymmetry (BIA) of WZ structure, is correctly described by the $k$-dependent SOC term, often neglected in the literature. Calculating the spin expectation value for the Bloch states, we find a Rashba-like spin texture with either clockwise (CW) or counterclockwise (CCW) orientation. All these spin-dependent features extracted from our $k.p$ Hamiltonian and parameter sets were systematically checked to agree with $ab$ initio calculations. Furthermore, based on our effective 8×8 Hamiltonian, we calculated the density of states (DOS) and predict the carrier density as a function of the Fermi energy. We also provide an analytical description of conduction band valid close to $\Gamma$ point and a compact description of the valence band ($6 \times 6$ Hamiltonian). But, we would like to emphasize that the best description of InAs and InP WZ is obtained using the total 8×8 Hamiltonian. In summary, the main goal of our paper is to provide a realistic $k.p$ description that can be used to study charge and spin transport, optics, as well as (superconducting) proximity effects in semiconductor heterostructures, e.g., quantum wells and wires. Such heterostructures cannot be investigated by first principles due to their mesoscopic sizes, and $k.p$ technique (using the prescription $\vec{k} \rightarrow -i\vec{\nabla}$) is currently perhaps the best choice for obtaining physically relevant quantities for them.

This paper is organized as follows: in Sec. II we present the $ab$ initio band structure of InAs and InP WZ. The multiband $k.p$ model and its considerations are discussed in Sec. III. In Sec. IV, we describe our main results: (i) the fitting approach; (ii) the comparison between the $ab$ initio and $k.p$ for band structure and the spin splittings; (iii) the spin expectation value for all energy bands and (iv) the DOS extracted from the 8×8 Hamiltonian. The analytical description of CB close to $\Gamma$ point is presented in Sec. V and the compact form of valence Hamiltonian, along with its parameters, is shown in Sec. VI. Finally, in Sec. VII we present our conclusions and possible direct applications of our effective multiband model.

II. $AB$ INITIO BAND STRUCTURE

The $ab$ initio electronic structure for InAs and InP in WZ phase was calculated within the density functional theory (DFT) framework, using the full potential linearized augmented plane wave method implemented by the WIEN2k code. To account for local and semilocal functional deficiencies to correctly describe band gaps in semiconductors, we used an efficient and accurate alternative for electronic structure calculations based on the modified Becke-Johnson (mBJ) exchange potential with LDA (local density approximation) correlation. It has been shown that the semilocal mBJ exchange potential provides prediction of band gaps of the same order as hybrid functionals and GW method. In addition, the semilocal approach to the exchange-correlation functional is barely expensive when compared to the LDA or the generalized gradient approximation. The SOC is included within the second variational step. Regarding the technical details of our calculations, we expanded the wave functions in atomic spheres for orbital quantum numbers up to 10; the plane wave cut-off multiplied with the smallest atomic radii equals to 10 and the irreducible Brillouin zone was sampled with 600 $k$ points. Further details on $ab$ initio calculations of III-V semiconductors, either with ZB or WZ structure, using the mBJ potential can be found in Ref.

![Figure 1](https://via.placeholder.com/150)

Figure 1: (Color online) $ab$ initio band structure along high-symmetry lines for (a) InAs and (b) InP in WZ phase. The inset shows the FBZ of WZ structure indicating the high-symmetry points. The rectangles highlight the region of interest around the $\Gamma$ point.

The particular order of cation (In) and anions (As, P) within the unit cell determines spin orientation. We consider the following primitive basis vectors for corresponding hexagonal Bravais lattice, $\vec{a}_1 = a(\sqrt{3}, -1, 0)/2$, $\vec{a}_2 = a(0, 1, 0)$, and $\vec{a}_3 = c(0, 0, 1)$, where $a$ and $c$ are the WZ lattice parameters. Using the three basis vec-
tors $\vec{a}_i$ ($i = 1, 2, 3$) we define the following four atomic positions that form the WZ structure: $(2/3, 1/3, u)$ and $(1/3, 2/3, 1/2 + u)$, with $u = 0$ for anion and $u = 3/8$ for cation. We note that in general there might be $u = 3/8 + \epsilon$ with a small dimensionless cell-internal structural parameter $\epsilon$ describing a deviation from ideal tetrahedrons as one observes for SiC polytypes.\textsuperscript{25,26} In our calculations we considered $\epsilon = 0$ since it is a rather small valued parameter.\textsuperscript{25,26} For the lattice parameters we considered $a = 4.2742$ Å and $c = 7.025$ Å for InAs and $a = 4.1148$ Å and $c = 6.7515$ Å for InP.

We show the band structures obtained with WIEN2k in Fig. 1(a) for InAs and Fig. 1(b) for InP. Both compounds show a direct band gap at $\Gamma$ point with values of $E_g = 0.467$ eV for InAs and $E_g = 1.494$ eV for InP. Due to the hexagonal symmetry of WZ, the $\Gamma$ point, as well as the symmetry line connecting $\Gamma$-A (hexagonal axis), belong to $C_{6v}$ symmetry group,\textsuperscript{27} that has only two dimensional double group representations. From this follows that the states along the hexagonal axis are spin degenerate.\textsuperscript{24,25,27,28} Irreducible representations of other points in the FBZ compatible with spin are singly degenerate. Hence, except for accidental or time-reversal degeneracies at $\Gamma$ and $A$ points, spin splittings must occur for all bands.

In Figs. 2(a), for InAs, and 2(b), for InP, we display the rectangular regions of Fig. 1 i. e., a zoom of the band structure around $\Gamma$ point. At this energy range, the anti-crossings and spin splittings features of the band structures are evident. Because of InAs large SOC, the valence band energy levels are further apart than InP bands and additional curvatures are present along $k_z$ direction. For InP the top two valence bands along $k_z$, shows similar curvatures and no anti-crossing is visible. The effect of SOC in the energy bands at $\Gamma$ point is shown schematically in Fig. 2(c). Without SOC, the irreducible representations belong to the simple group, while with SOC, they are referred as double group. This distinction is important for $k.p$ perturbative approaches.

We present a comparison between our ab initio calculations and other theoretical papers of the literature in table I. Besides the lattice constants $a$ and $c$ we compare the values of the internal parameter $u$, the energy gap $E_g$, and the energy difference between the top valence band $\Gamma_9$ to the other bands $\Gamma_7$ and $\Gamma_7'$ [following the notation of Fig. 2(c)]. These energy differences are defined as $\Delta E_{97} = E(\Gamma_9) - E(\Gamma_7)$ and $\Delta E'_{97} = E(\Gamma_9) - E(\Gamma'_7)$. It is very common to compare the crystal field splitting energy, $\Delta_1$, and the SOC energy, $\Delta_{SO}$ however, these parameters are usually obtained under the quasicubic approximation and do not provide a direct comparison with experiments such as $\Delta E_{97}$ and $\Delta E'_{97}$. We can see that all the values obtained by our calculations are within the range of reported data in previous papers. We also compare experimental measurements of the energy gap with our calculated values, shown in table I. We focused on experimental data obtained by photoluminescence measurements at low temperature of large diameter nanowires, so that lateral quantum confinement is negligible. For both InAs (despite the reduced set of available data) and InP compounds, our calculated values of the energy gaps are consistent with the experiments. Furthermore, photoluminescence excitation measurements can probe the $\Gamma_7$ and $\Gamma_7'$ valence bands and allow us to check our calculated values for $\Delta E_{97}$ and $\Delta E'_{97}$ energies. To the best of our knowledge, such experiments are only available for InP. Typical values found for $\Delta E_{97}$ and $\Delta E'_{97}$ in InP WZ are: 0.044 eV and 0.187 eV in Ref. 9; 0.043 eV and 0.179 eV in Ref. 56; and 0.044 eV and 0.182 eV in Ref. 57. Our calculated values for InP of $\Delta E_{97}$ = 0.0354 eV and $\Delta E'_{97}$ = 0.145 eV (from table I), are also in good agreement with these experimental trends. For completeness, we provide in appendix A the calculated values of effective masses around $\Gamma$-point.

### III. $k.p$ FORMULATION

One alternative approach to ab initio band structure calculations is the $k.p$ method. In the $k.p$ approach, the many-body interactions of electrons with nuclei and other electrons are described by an effective potential which has the same periodicity as the Bravais lattice of the crystal.\textsuperscript{28} Such periodic property of the potential allows us to use Bloch’s theorem for the total wave function.
The single-particle Hamiltonian for the periodic part of the Bloch function, $u_{n,k}(\vec{r})$, can be written as:

$$
H = \frac{p^2}{2m_0} + V(\vec{r}) + \frac{\hbar}{4m_0c^2} \left[ \nabla V(\vec{r}) \times \vec{p} \right] \cdot \vec{\sigma} 
$$

$$
+ \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0} \vec{k} \cdot \vec{p} + \frac{\hbar^2}{4m_0c^2} \left[ \nabla V(\vec{r}) \times \vec{k} \right] \cdot \vec{\sigma},
$$

in which the different terms in the Hamiltonian are identified for convenience.

We can solve the above equation perturbatively expanding the functions $u_{n,k}(\vec{r})$ around a specific reciprocal space point that we know the solutions for the Hamiltonian. Since WZ InAs and InP have a direct band gap at $\Gamma$ point, this is the chosen expansion point. The perturbative technique we use in this paper is Löwdin’s formalism. In this approach, the functions at $\Gamma$ point, i.e., the basis set to expand $u_{n,k}(\vec{r})$, are divided into classes A and B. The energy bands we are interested in describing comprise the class A while the other energy bands belong to class B. The contribution of states in class B appear in second or higher orders of perturbation. The matrix elements we consider can arise from first or second order perturbation, reading as

$$
H_{f,\alpha\alpha'}^{(1)} = \langle \alpha | H_f | \alpha' \rangle,
$$

and

$$
H_{g,\alpha\alpha'}^{(2)} = \sum_{\beta} \frac{\langle \alpha | H_f | \beta \rangle \langle \beta | H_g | \alpha' \rangle}{E_{\alpha\alpha'} - E_\beta},
$$

where $H_f$ and $H_g$ can be any of the terms of equation (1), except $H_0$.

### Table I: Comparison of theoretical data for InAs and InP in WZ phase.

| Material | Study       | $a$ (Å) | $c$ (Å) | $u$ (Å) | $E_g$ (eV) | $\Delta E_{97}$ (eV) | $\Delta E_{97}'$ (eV) |
|----------|-------------|---------|---------|---------|------------|----------------------|----------------------|
| InAs     | This study  | 4.2742  | 7.0250  | 0.3750  | 0.4670     | 0.0592               | 0.3527               |
|          | Ref. 23     | 4.1505  | 6.7777  | 0.3750  | 0.4810     | 0.1050               | 0.4960               |
|          | Ref. 25     | 4.2570  | 6.9894  | 0.3747  | 0.4810     | 0.0573               | 0.3937               |
|          | Ref. 27     | 4.2564  | 7.0046  | 0.3740  | 0.4610     | 0.0700               | 0.3640               |
|          | Ref. 47     | 4.2472  | 7.0250  | 0.3742  | 0.4610     | 0.0660               | 0.3600               |
| InP      | This study  | 4.1148  | 6.7515  | 0.3750  | 1.4940     | 0.0354               | 0.1450               |
|          | Ref. 23     | 4.2839  | 6.9055  | 0.3750  | 1.4740     | 0.0630               | 0.3480               |
|          | Ref. 24     | 4.1500  | 6.9120  | 0.3710  | 1.4936     | 0.0450               | 0.2430               |
|          | Ref. 25     | 4.1148  | 6.7515  | 0.3745  | 1.5760     | 0.0321               | 0.1339               |

$a$, $c$ and $u$ from Ref. 53.

### Table II: Comparison between theoretical and experimental values of the energy gap.

| Material | $E_g$ (eV) | $E_g$ (eV) |
|----------|------------|------------|
|          | This study | Experiment |
| InAs     | 0.467      | 0.520 (7 K)$^a$, 0.500 (20 K)$^b$ |
|          |            | 0.458 (5 K)$^c$ |
| InP      | 1.494      | 1.492 (10 K)$^d$, 1.494 (10 K)$^e$ |
|          |            | 1.490 (20 K)$^f$, 1.491 (4 K)$^g$ |
|          |            | 1.493 (4 K)$^h$, 1.488 (6 K)$^i$ |

$a$Ref. 60, $b$Ref. 61, $c$Ref. 62, $d$Ref. 57, $e$Ref. 60, $f$Ref. 63, $g$Ref. 3, $h$Ref. 64, $i$Ref. 9

Since the unperturbed term, $H_0$, in Eq. (1) does not contain SOC effects explicitly, we consider the simple group description of the energy bands, the most usual approach in the literature. Under such approximation, the states in class A belong to the irreducible representations shown in the left side of Fig. 2(c), a 4 dimensional Hilbert space, combined with the spin 1/2 angular momentum, a 2 dimensional Hilbert space. Therefore, the 8 dimensional basis set for the $k.p$ Hamiltonian in Dirac notation is given by:

$$
|c_1\rangle = -\frac{\Gamma_5^z + i\Gamma_5^y}{\sqrt{2}} \quad |c_5\rangle = -\frac{\Gamma_5^z + i\Gamma_5^y}{\sqrt{2}}
$$

$$
|c_2\rangle = \frac{\Gamma_5^x}{\sqrt{2}} \quad |c_6\rangle = |\Gamma_1^y \rangle
$$

$$
|c_3\rangle = |\Gamma_1^x \rangle \quad |c_7\rangle = i |\Gamma_1^x \rangle
$$

$$
|c_4\rangle = \frac{\Gamma_5^x - i\Gamma_5^y}{\sqrt{2}} \quad |c_8\rangle = i |\Gamma_1^y \rangle,
$$

with 1-6 representing the valence band states and 7-8 the
conduction band states. Since $\Gamma_{5c}$ is two dimensional, we identified its basis states by $|\Gamma_{5c}^x\rangle \sim x$ and $|\Gamma_{5c}^y\rangle \sim y$. The single arrows ($\uparrow, \downarrow$) represent the projection of spin up and spin down, eigenvalues of $\sigma_z$ Pauli matrix. The states in class B have simple group symmetries $\Gamma_1$, $\Gamma_3$, $\Gamma_5$, and $\Gamma_6$, which is the only necessary information to calculate second order contributions.

$$E_c - \Delta_1, \quad |c_1\rangle \quad |c_2\rangle \quad |\Delta_1\rangle \quad |c_3\rangle \quad |c_4\rangle \quad |c_5\rangle \quad |c_6\rangle$$

Figure 3: (Color online) Possible interactions of the Hamiltonian terms (a) $H_0$, (b) $H_{SO}^{(1)}$, (c) $H_{kp}^{(1)}$, (d) $H_{kSO}^{(1)}$, and (e) $H_{kp}^{(2)}$. The arrows on top of panel (a) indicate spin up and spin down projections of the basis states. Since $|c_1(4)\rangle$ and $|c_2(5)\rangle$ are degenerate, we indicate the interactions arising from $|c_1(4)\rangle$ with solid lines and the interactions arising from $|c_2(5)\rangle$ with dashed lines. For the other states without degeneracy we used solid lines. In panel (a) we show the energy splittings without SOC, formally defined in Appendix B.

To describe the interaction among the energy bands, we consider all terms of equation 1, in first order perturbation and only the term $H_{kp}$ in second order. Therefore, the total matrix Hamiltonian in the basis set |11\rangle comprises the following terms

$$H = H_0 + H_{SO}^{(1)} + H_{kp}^{(1)} + H_{kSO}^{(1)} + H_{kp}^{(2)} \quad (5)$$

with the explicit form of each matrix and the definition of the parameters given in the Appendix B.

In Fig. 3 we show schematically the interactions for each term in the total Hamiltonian |1]. The panel 3(a) represents the unperturbed Hamiltonian without SOC, where states $|c_1(4)\rangle$ and $|c_2(5)\rangle$ are degenerate for spin up (down). The only terms that couple different spin projections arise from $H_{SO}^{(1)}$ or $H_{kSO}^{(1)}$, panels |3b| and |3d|, respectively. Usually $H_{kp}^{(1)}$ is neglected in WZ Hamiltonians.28,29,31,67–70 However, the explicit interactions for non-zero $k$-values are crucial to correctly describe the spin splitting properties. We included $H_{kSO}^{(1)}$ following the approach of Dresselhaus for ZB. Moreover, the coupling of $H_{SO}^{(1)}$ to other terms provides additional contributions to the spin splitting of energy bands. Besides spin splitting properties, we want a good description of the band structure curvatures. Such effects can be modeled by linear and quadratic terms of the $H_{kp}^{(1)}$ and $H_{kp}^{(2)}$, panels |3c| and |3e|, respectively. The only term that allows a $k$-dependent self interaction of states is $H_{kp}^{(2)}$ which gives the effective mass contribution to our model.

Although the $k.p$ method provides the functional form of the Hamiltonian, the parameters that describe different materials cannot be found by group theory arguments only. In order to calculate the matrix elements we would need the functions at the expansion point and also the periodic potential $V(\mathbf{r})$. Alternatively, we can directly fit the $k.p$ Hamiltonian to the $ab\text{ initio}$ band structure to extract the parameters 29,31,67–72.

IV. NUMERICAL FITTING OF THE 8×8 k.p HAMILTONIAN

We start our fitting approach by calculating the $k$-independent parameters of the Hamiltonian, i. e., the energy splittings. The values for crystal field splitting, $\Delta_1$, and the conduction band energy, $E_c$, can be obtained from the $ab\text{ initio}$ calculation without SOC, which is in fact the assumption of the $k.p$ perturbative theory $[H_0$ term, see Fig 3(a)]. This approach is very useful because it simplifies the calculation of the SOC energy splittings inside valence band, $\Delta_2$ (coupling same spins) and $\Delta_3$ (coupling different spins), and the SOC between conduction and valence bands, $\Delta_4$. Please refer to appendix B for the formal definition of these splitting energies. By setting the values of $\Delta_1$ and $E_c$, it possible to have $\Delta_2 \neq \Delta_3$ and neglect the cubic approximation.23–25 If the values of $\Delta_1$ and $E_c$ were not found without SOC, we would have to determine 5 variables having only 3 linear independent combinations of the energy bands with SOC. This approach would provide a range of possible values and further analysis would be necessary. Starting with $\Delta_1$ and $E_c$ values without SOC, we obtained four different solution sets for the SOC splitting energies since $\Delta_1$ and $\Delta_2$ are off-diagonal terms in the Hamiltonian and can assume positive or negative values with same magnitude. At $\Gamma$ point any of these solution sets give the same eigenvalues, therefore we set $\Delta_1$ to be positive23–25,27 and investigated the effect of positive and negative values of $\Delta_4$.

Before starting the fitting of the $k$-dependent parameters, it is important to define the fitting region we are
interested in, which is connected to the limits of our \( \mathbf{k.p} \) model. Basically, in order to describe as precisely as possible the 8 bands we are interested in, we should stay in a region away from the influence of remote bands, roughly \( k \sim 1.5 \text{ nm}^{-1} \), see Fig. 2(a)-(b). We also want to have a nice description of the anti-crossings in the bands structure around \( k \sim 0.5 \text{ nm}^{-1} \). Furthermore, in the \( \mathbf{k.p} \) Hamiltonian \( k_x \) and \( k_y \) directions are equivalent, but this is not the case for the \textit{ab initio} band structure. Around \( k \sim 1.0 \text{ nm}^{-1} \), the \textit{ab initio} band structures along \( \Gamma-K \) and \( \Gamma-M \) directions are different, especially the spin splitting, which is another feature to be described. Therefore, it is reasonable to set the goal of our fitting at \( k = 1.0 \text{ nm}^{-1} \) to find the best parameters set that describes the \textit{ab initio} band structure around \( \Gamma \) point for all the 8 bands.

To increase the accuracy of our parameter sets, we fitted, simultaneously, the energy bands in multiple directions of the FBZ (\( \Gamma-K, \Gamma-M, \Gamma-A, \Gamma-H \) and \( \Gamma-L \)). The fitting algorithm was developed using the LMFIT package of python assuming several minimization methods available. We noticed that the minimization methods behave differently and usually provide different parameter sets. After an initial fit, we chose the best parameter set and used it as input for a new fit using all minimization methods again. To find the best fit, the band structures and spin splittings are compared by their residue up to \( k = 1.0 \text{ nm}^{-1} \) for all directions. The best parameter sets for InAs and InP found by our fitting approach are presented in Table III.

In Fig. 4, we present the comparison between the fitted and WIEN2k \textit{ab initio} band structures along \( k_x \) and \( k_z \) for InAs and InP. All the important features around \( \Gamma \) point, i.e., anti-crossings and spin splittings, are captured by our model. We notice a good agreement up to \( k = 1.0 \text{ nm}^{-1} \) with small deviations above it, indicating that we are reaching the region where the influence of remote energy bands becomes important. We labeled the valence bands according to the composition of states at \( \Gamma \) point. Following Chuang and Chang’s notation, \( HH \) is pure composed of \( |c_{1(4)}⟩ \) states, \( LH \) has more contribution from \( |c_{2(5)}⟩ \) than \( |c_{3(6)}⟩ \) states, and \( CH \) has more contribution from \( |c_{3(6)}⟩ \) than \( |c_{2(5)}⟩ \) states. Since this analysis is usually performed without \( \Delta_4 \) parameter, we also calculated \( \Delta_2 \) and \( \Delta_3 \) considering \( \Delta_4 = 0 \) and we found that the same labeling holds (this values are shown in Sec. VI). Furthermore, we also compared the \( \mathbf{k.p} \) composition with the projection to atomic orbitals of the \textit{ab initio} wave functions and the same trends can be noticed. The labeling order of CH-LH in InAs is due to the values of SOC splitting energies, which are slightly larger than the crystal field splitting. For InP, the crystal field splitting is dominant leading to LH-CH ordering. Although this labeling of the valence band can be confusing, it is very useful to extract optical trends from the band-edge transitions. For instance, if we take into account optical transitions arising from the top two valence bands, we can expect InP light polarization to be more in-plane due to LH contribution than InAs due to CH contribution. Finally, for the conduction band of both InAs and InP we simply label it CB, short notation for conduction.
band; CB is mainly composed of $|c_7(s_1)\rangle$ states.

Let us take a closer look at the spin splitting properties obtained from the $\mathbf{k}.\mathbf{p}$ model and the ab initio. We show the comparison between the two methods in Fig. 5 for InAs and InP along $k_x$ direction. Similar to the band structure, we have a good agreement up to $k = 1.0$ nm$^{-1}$ with deviations above this region. The intricate behaviors, i.e., the appearance of maxima and crossings between HH spin split bands are also described by our model. All these spin splitting characteristics have only one physical origin, the BIA of WZ structure. The strength of SOC is greater in InAs than InP, visible at the peak values and positions. From the largest to the smallest values of the spin splitting, we have CH (LH), LH (CH), CB and HH for InAs (InP). Furthermore, a linear behavior is maintained for InP CB throughout the fitting region. For InAs, this linear behavior is attained only in a small region close to $\Gamma$ point. In appendix C, we present the band structure and spin splittings for the other FBZ directions used in the fitting.

Another feature we investigated is the spin orientation, i.e., the spin expectation value, $\langle \vec{\sigma} \rangle$, for the different energy bands, presented in Fig. 6 for the $k_xk_y$ plane ($k_z = 0$). We chose the constant-energy contours to be $E_n(k_x = 0.5$ nm$^{-1}, k_y = 0, k_z = 0)$ of the outer branch, i.e., $E_{CB} \sim 630.0$ meV, $E_{HH} \sim -37.2$ meV, $E_{CH} \sim -123.0$ meV, $E_{LH} \sim -391.8$ meV for InAs and $E_{CB} \sim 1563.5$ meV, $E_{HH} \sim -21.9$ meV, $E_{LH} \sim -75.0$ meV, $E_{CH} \sim -156.7$ meV for InP. We found that all the investigated energy bands show a Rashba-like spin texture. For InAs, the bands CB, HH and CH have the same spin texture, i.e., CW (CCW) orientation for the inner branches and in gray for the outer branches.
(outer) branch, while LH has the CWW (CW) orientation for the inner (outer) branch. In other words, the top two valence bands have the same spin texture while the third valence band have the opposite. For InP, the same spin texture holds, even though the labeling of CH and LH is reversed. The spin textures calculated with the kp model were also checked with the ab initio calculations.

Performing the fitting approach with the negative sign of $\Delta_4$ we obtained the same behavior of the band structure and the spin splittings, but with a reversed orientation in the spin texture, i.e., CW orientation becomes CCW and vice-versa for all bands. Specifically, we found that starting with negative value of $\Delta_4$, the signs of parameters $A_7$, $\alpha_1$, $\alpha_2$, $\alpha_3$, $\gamma_1$, $B_1$, $B_2$ and $B_3$ are changed, but not their amplitude. This change in the spin texture is a feature expected from ab initio regarding the cation and anion positions within the crystal unit cell and it is reflected in our kp model and parameters. Therefore, in order to provide reliable parameter sets for kp Hamiltonians, not only the band structure and the spin splittings should be checked but also the spin orientation. We would like to emphasize that all these features were systematically checked in this study.

A. Density of states and carrier density

Relying on the effective 8x8 kp Hamiltonian, it is straightforward to calculate a smooth DOS using a fine 3-dimensional (3D) mesh of $k$ points (300 × 300 × 300) without much computational effort. In Fig. 7(a) we show the DOS for the conduction band of InAs and InP. For comparison, we also show the DOS for the 3D parabolic band model $\text{DOS}(E) \propto \sqrt{E}$, which is just a straight line in the log-log scale. Due to the complex behavior of the InAs and InP conduction bands, we clearly see deviations from the linear behavior, especially for InAs. For the DOS of the valence band, presented in Fig. 7(b) the deviations from the parabolic model are much more visible, showing explicitly the need of a multiband approach. When the valence band energy approaches the CH (LH) region of InAs (InP), the DOS changes its curvature. Moreover, the valence band DOS is approximately one order of magnitude larger than the DOS of the conduction band, a behavior attributed to the small curvatures of the valence bands, i.e., large effective masses for holes (in a single band picture). Integrating the DOS we obtain the carrier density as a function of the Fermi energy, $E_f$. For instance, for 100 meV above the energy gap $\sim 1.6 \times 10^{18}$ cm$^{-3}$ for InAs and $\sim 6.5 \times 10^{18}$ cm$^{-3}$ for InP. The solid vertical lines in Figs. 7(b) and (d) indicate the LH energy at Γ-point for InP while the dashed vertical lines indicate the CH energy at Γ-point for InAs.

V. ANALYTICAL DESCRIPTION FOR CONDUCTION BAND

Since the conduction band has a predominant contribution of $|c_{7(8)}\rangle$ states, it is useful to provide an analytical description that holds for small regions close to the Γ point that can be easily used in spin dynamics studies. We apply the Löwdin’s approach again, but now dividing the basis states $\Lambda$ (Eq. 4) of the full matrix into new two classes $\Lambda'$ ($|c_{7,8}\rangle$) and $\Lambda''$ ($|c_{1,\ldots,6}\rangle$). Using only the terms we already calculated in the full Hamiltonian as contribution to the effective Hamiltonian, this Löwdin’s approach is usually refereed to as folding down. The effective Hamiltonian for the first order folding down, keeping terms up to $k^3$ can be written as

$$H_{\text{CB}} = M(\vec{k}) \mathcal{I}_2 + \vec{\Omega}(\vec{k}) \cdot \vec{\sigma},$$

in which $\mathcal{I}_2$ is a 2x2 identity matrix and $M$ is the effective mass term given by

$$M = E_g + m_z k_z^2 + m_{xy} (k_x^2 + k_y^2),$$
with the coefficients $m_z$ and $m_{xy}$ given by

$$m_z = e_1 + \frac{P_2^2}{E_c} + \frac{2\beta_1^2}{E_c - \Delta_1 + \Delta_2} + \frac{2\Delta_4^2(A_1 + A_3)}{(E_c - \Delta_1 + \Delta_2)^2},$$

$$m_{xy} = e_2 + \frac{1}{2}\left(\frac{P_2 + \beta_1}{E_c - \Delta_1 + \Delta_2}\right)^2 + \frac{1}{2}\left(\frac{P_2 - \beta_1}{E_c - \Delta_1 + \Delta_2}\right)^2 + \frac{\beta_2^2}{E_c - \Delta_1 + \Delta_2}. \tag{8}$$

The SOC field $\tilde{\Omega}(\vec{k})$ is written as

$$\tilde{\Omega}(\vec{k}) = \begin{bmatrix} \alpha + \gamma_z k_y^2 + \gamma_{xy} (k_x^2 + k_y^2) \\ -k_x \\ 0 \end{bmatrix}, \tag{9}$$

with linear and cubic coefficients given by

$$\alpha = -\gamma_1 + \frac{2\Delta_4(P_2 + \beta_1)}{E_c - \Delta_1 + \Delta_2},$$

$$\gamma_z = 2\sqrt{2}\beta_1 B_3 \left(\frac{2\beta_1 B_1}{E_c} + \frac{2\Delta_4(P_2 + \beta_1)(A_1 + A_3)}{(E_c - \Delta_1 + \Delta_2)^2}\right),$$

$$\gamma_{xy} = -\frac{2\beta_2 B_2}{E_c} + \frac{2\Delta_4(P_2 + \beta_1)(A_2 + A_4)}{(E_c - \Delta_1 + \Delta_2)^2} \tag{10}.$$ 

This analytical approach for the conduction band provides a reasonable description up to 0.2 nm$^{-1}$ for InAs and 0.6 nm$^{-1}$ for InP, which is roughly 100 meV above the energy gap in both cases. The numerical values of $m_z$, $m_{xy}$, $\alpha$, $\gamma_z$ and $\gamma_{xy}$ can be obtained by replacing the parameters with values presented in Table III. Setting the $k$-dependent SOC parameters $\gamma_1$ and $\beta_1$ to zero, we recover the analytical linear splitting found in Ref. [28]. Our approach has the advantage of also providing the analytical description of the cubic terms. For additional corrections to the cubic term, it is possible to include higher order terms in the folding down approach. The comparison to \textit{ab initio} data using the analytical expressions presented in this section can be found in the supplemental material.

\section{VI. COMPACT DESCRIPTION FOR VALENCE BAND}

Because of the coupling from the crystal field and SOC energies, the best simplified description for the valence band is simply neglecting the coupling with conduction band, thus leading to a 6×6 matrix. It is possible to write this 6×6 Hamiltonian in a compact form using direct products of 3×3 (orbital) and 2×2 (spin) matrices. In the basis set $\{|e_1\}, \{|e_3\}, \{|e_2\}, \{|e_5\}, \{|e_6\}, \{|e_4\}\}$, the compact form of valence band is written as

$$H_{\text{VB}} = \Delta_1 J_x^2 I_2 + \Delta_2 J_y \sigma_z + \sqrt{\Delta_3}(J_x \sigma_- + J_- \sigma_+ + (A_1 I_3 + A_3 J_x^2)k_x^2 I_2 + (A_2 I_3 + A_4 J_x^2)(k_x^2 + k_y^2) I_2 - A_5 J_x^2 k_y^2 I_2 - 2A_6 k_z(\{J_z, J_+\} k_+ + \{J_z, J_-\} k_-) I_2 + iA_7 (J_+ k_- - J_- k_+) I_2 + i\sqrt{2} \alpha_1 \{J_x, J_y\} (\sigma_z k_+ - 2\sigma_+ k_z) - \{J_x J_+\}(\sigma_+ k_- - 2\sigma_- k_z) + i(\alpha_3 - \alpha_2) J_y^2 - \alpha_3 I_3 (\sigma_+ k_- - \sigma_- k_+) \tag{11}.$$

with $\{J_x J_y\} = \frac{1}{2}(J_x J_y + J_y J_x)$, $J_{\pm} = \frac{1}{\sqrt{2}}(J_x \pm J_y)$, $\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm \sigma_y)$ and $k_{\pm} = k_x \pm ik_y$. The definitions of $J_x, J_y$ and $J_z$ matrices can be found in appendix A (eq. A3) of Ref. [28]. The matrix $I_n$ is a $n$-dimensional identity. The product of 3×3 matrices ($A$) with 2×2 matrices ($a$) is defined here as

$$Aa = \begin{bmatrix} a_{11}A & a_{12}A \\ a_{21}A & a_{22}A \end{bmatrix}. \tag{12}$$

Table IV: Parameter sets of the 6×6 valence band Hamiltonian for InAs and InP WZ. The units follow Table III

| Parameter | InAs | InP |
|-----------|------|-----|
| Energy splittings | | |
| $\Delta_1$ | 0.1003 | 0.0945 |
| $\Delta_2$ | 0.1038 | 0.0286 |
| $\Delta_3$ | 0.1037 | 0.0310 |
| Linear parameters | | |
| $A_7$ | -0.5565 | -0.0917 |
| $a_1$ | -0.0237 | 0.3309 |
| $a_2$ | -0.0758 | -0.0702 |
| $a_3$ | -0.0967 | -0.0521 |
| Second order parameters | | |
| $A_1$ | -17.2689 | -10.5414 |
| $A_2$ | -1.2047 | -1.4542 |
| $A_3$ | 16.6637 | 9.4589 |
| $A_4$ | -7.6202 | -3.2741 |
| $A_5$ | -5.9281 | 3.9468 |
| $A_6$ | -7.3872 | -0.2759 |

To obtain the best parameter sets that describe the \textit{ab initio} band structure, we performed the same fitting approach described in section IV. We found that, in order to attain the monotonic behavior of the bands, some features of the band structure or the spin splittings are not matched as precisely as the results using the 8×8 Hamiltonian. For instance, the band structures and the spin splittings for InP looks reasonable, however, the spin
VII. CONCLUSIONS

In this paper, we have calculated the band structure of InAs and InP in WZ phase using the WIEN2k \textit{ab initio} code. Both compounds have a direct band gap at \( \Gamma \) point with the SOC effects clearly larger for InAs than InP. Our calculations are consistent with theoretical and experimental reported values in the literature. In order to describe the band structure around the FBZ center, we developed a multiband \( 8 \times 8 \) \textit{k.p} model for the first conduction band and the top three valence bands, including spin. The fitted parameters we obtained for the \textit{k.p} Hamiltonian recover the important features of the \textit{ab initio} band structure with good agreement up to 1.0 nm\(^{-1}\) for multiple directions in the FBZ. Due to the stronger SOC of InAs compared to its crystal field splitting, the labeling of LH and CH energy bands at \( \Gamma \) point is reversed from InP. Regarding the spin splitting properties, we included the \( k \)-dependent SOC term in the Hamiltonian, which is usually neglected in the literature. This term, combined with the other indirect couplings in the Hamiltonian, allowed the description of the spin splitting properties further away from the vicinity of \( \Gamma \) point. Our model captured all the important features including the description of maxima values and also the crossing between the spin split bands (clearly seen in HH band of InP, for instance). All these intricate behaviors of spin splitting have a unique physical origin, the BIA of the WZ structure. Furthermore, we calculated the in-plane spin orientation, i.e., the spin expectation value, of the energy bands and found that they all have a Rashba-like spin texture, either CW or CCW. This spin orientation was also compared to \textit{ab initio} data to correctly identify the signs of the parameters in the Hamiltonian. Using our multiband \textit{k.p} Hamiltonian, we obtained the DOS for conduction and valence bands and calculated the carrier density as function of the Fermi energy. In addition to the \( 8 \times 8 \) Hamiltonian, we present analytical expressions for the effective masses and the SOC field of conduction band which holds in the vicinities of the \( \Gamma \) point. For completeness, we also fitted the \( 6 \times 6 \) \textit{k.p} model for valence band to the \textit{ab initio} data. We emphasize that the best effective description that matches our \textit{ab initio} calculations is the full \( 8 \times 8 \) \textit{k.p} Hamiltonian.

In conclusion, we provided in this study robust \textit{k.p} models and parameter sets that can be straightforwardly applied to investigate novel effects in InAs- and InP-based nanostructures. For instance, polytypic systems of mixed WZ and ZB are already demonstrated experimentally for both InAs and InP with great growth control of the different phases\cite{26,27} and there are also theoretical models to treat such systems.\cite{28,29} Furthermore, InAs nanowires are also a platform for studies in Majorana fermions\cite{30}. One of the key ingredients for such realization is the presence of a robust SOC to split the energy bands, a feature already included in our model. Finally, it is straightforward to included strain effects by using the well established WZ strain Hamiltonian\cite{38,39} combined with the elastic constants and deformation potentials for InAs and InP in WZ phase already reported in the literature\cite{20,21,77,79}.

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Appendix A: effective masses

Very close to \( \Gamma \)-point we can estimate the effective masses by fitting a parabolic dispersion to the \textit{ab initio} data. In table \ref{table:effective_masses} we show the values of effective masses along \( k_z \) and \( k_x \) directions for the highlighted energy bands of Figs. 2(a)-(b). For \( k_x \) direction, we calculated the effective masses assuming the average value of the spin splitting bands, i.e., \((E_o + E_i) / 2\) with the subindex \( o (i) \) indicating the outer (inner) branch.

Table V: Effective masses for InAs and InP along \( k_z \) (\( m_\|^* \)) and \( k_x \) (\( m_\perp^* \)) for the highlighted bands of Fig. 2(a)-(b). The effective masses were obtained by fitting a parabola up to 2\% of the FBZ along the specified directions.

|        | InAs     | InP      |
|--------|----------|----------|
| \( m_\parallel^* \) | 0.0370 | 0.0947   |
| \( m_\perp^* \)   | 0.0416 | 0.1183   |
| \( m_o^* \)       | -0.9738| -1.0646  |
| \( m_i^* \)       | -0.1046| -0.2091  |

For completeness, we also fitted the \( 6 \times 6 \) \textit{k.p} model for valence band to the \textit{ab initio} data. We emphasize that the best effective description that matches our \textit{ab initio} calculations is the full \( 8 \times 8 \) \textit{k.p} Hamiltonian.
Appendix B: Hamiltonian terms and parameters

In this appendix, we present the matrix forms of all terms in equation (3) and the definition of parameters using the simple group formalism.

Matrix representation of $H_0$:

$$H_0 = \text{diag} [\Delta_1, \Delta_1, 0, \Delta_1, \Delta_1, 0, E_c, E_c] ,$$

(13)

with the definitions $\langle \Gamma_{5v}^x | H_0 | \Gamma_{5v}^z \rangle = \langle \Gamma_{5v}^y | H_0 | \Gamma_{5v}^y \rangle = \Delta_1$, $\langle \Gamma_{1v} | H_0 | \Gamma_{1v} \rangle = 0$ and $\langle \Gamma_{1c} | H_0 | \Gamma_{1c} \rangle = E_c$.

Matrix representation of $H_{SO}^{(1)}$:

$$H_{SO}^{(1)} = \begin{bmatrix}
\Delta_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\Delta_2 & 0 & 0 & \sqrt{2}\Delta_3 & 0 & 0 & -i\sqrt{2}\Delta_4 \\
0 & 0 & 0 & \Delta_2 & 0 & 0 & 0 & 0 \\
0 & 0 & \sqrt{2}\Delta_3 & 0 & -\Delta_2 & 0 & i\sqrt{2}\Delta_4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -i\sqrt{2}\Delta_4 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix} ,
$$

(14)

with the definitions

$$\Delta_2 = \frac{ih}{4m_0^2c^2} \left\langle \Gamma_{5v}^x \right\rangle \frac{\partial \Gamma_{5v}^x}{\partial p_y} \left( \frac{\partial \Gamma_{5v}^x}{\partial y} - \frac{\partial \Gamma_{5v}^x}{\partial p_x} \right),$$

$$\Delta_3 = \frac{ih}{4m_0^2c^2} \left\langle \Gamma_{5v}^y \right\rangle \frac{\partial \Gamma_{5v}^x}{\partial p_z} \left( \frac{\partial \Gamma_{5v}^x}{\partial z} - \frac{\partial \Gamma_{5v}^x}{\partial p_y} \right),$$

$$\Delta_4 = \frac{ih}{4m_0^2c^2} \left\langle \Gamma_{5v}^y \right\rangle \frac{\partial \Gamma_{5v}^x}{\partial p_y} \left( \frac{\partial \Gamma_{5v}^x}{\partial p_z} - \frac{\partial \Gamma_{5v}^x}{\partial z} \right).$$

Matrix representation of $H_{kp}^{(1)}$:

$$H_{kp}^{(1)} = \begin{bmatrix}
0 & 0 & iA_7 k_- & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} P_2 k_- & 0 \\
0 & 0 & -iA_7 k_+ & 0 & 0 & 0 & \frac{1}{\sqrt{2}} P_2 k_+ & 0 \\
-\frac{1}{\sqrt{2}} P_2 k_+ & iA_7 k_- & 0 & 0 & 0 & 0 & P_1 k_z & 0 \\
0 & 0 & iA_7 k_- & 0 & 0 & 0 & -iA_7 k_+ & 0 \\
0 & 0 & 0 & 0 & 0 & iA_7 k_- & 0 & \frac{1}{\sqrt{2}} P_2 k_+ \\
0 & 0 & 0 & iA_7 k_- & 0 & 0 & P_1 k_z & 0 \\
-\frac{1}{\sqrt{2}} P_2 k_- & \frac{1}{\sqrt{2}} P_2 k_- & P_1 k_z & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} P_2 k_- & -\frac{1}{\sqrt{2}} P_2 k_+ & P_1 k_z \\
\end{bmatrix} ,
$$

(16)

with the definitions

$$A_7 = \frac{i}{\sqrt{2} m_0} \left\langle \Gamma_{5v}^x \right\rangle \left( \frac{\partial \Gamma_{5v}^x}{\partial p_x} \right),$$

$$P_2 = \frac{ih}{m_0} \left\langle \Gamma_{5v}^x \right\rangle \left( \frac{\partial \Gamma_{5v}^y}{\partial p_y} \right),$$

$$P_1 = \frac{ih}{m_0} \left\langle \Gamma_{5v}^x \right\rangle \left( \frac{\partial \Gamma_{5v}^y}{\partial p_z} \right),$$

$$k_\pm = k_x \pm ik_y .$$

(17)
Matrix representation of $H_{kSO}^{(1)}$:

$$H_{kSO}^{(1)} = \begin{pmatrix}
0 & 0 & -\frac{i}{\sqrt{2}} \alpha_1 k_- & 0 & -i \alpha_2 k_- & 0 & \frac{1}{\sqrt{2}} \beta_1 k_- & 0 \\
0 & 0 & -\frac{i}{\sqrt{2}} \alpha_2 k_- & 0 & -i \alpha_2 k_- & 0 & \frac{1}{\sqrt{2}} \beta_1 k_- & 0 \\
\frac{1}{\sqrt{2}} \alpha_1 k_+ & \frac{1}{\sqrt{2}} \alpha_2 k_+ & 0 & 0 & -i \alpha_2 k_- & 0 & \frac{1}{\sqrt{2}} \beta_1 k_- & 0 \\
i \alpha_2 k_+ & 0 & i \sqrt{2} \alpha_1 k_- & 0 & -i \alpha_3 k_- & 0 & -\frac{1}{\sqrt{2}} \beta_1 k_- & 0 \\
i \alpha_2 k_+ & 0 & i \sqrt{2} \alpha_1 k_- & 0 & -i \alpha_3 k_- & 0 & -\frac{1}{\sqrt{2}} \beta_1 k_- & 0 \\
0 & -i \sqrt{2} \alpha_1 k_- & i \alpha_3 k_- & -\frac{i}{\sqrt{2}} \alpha_1 k_+ & -\frac{i}{\sqrt{2}} \alpha_2 k_+ & 0 & \beta_2 k_+ & 0 \\
0 & 0 & -i \sqrt{2} \alpha_1 k_- & -\frac{i}{\sqrt{2}} \alpha_2 k_+ & 0 & \beta_2 k_+ & 0 & -i \gamma_1 k_- \\
\frac{1}{\sqrt{2}} \beta_1 k_- & \frac{1}{\sqrt{2}} \beta_2 k_- & 0 & 0 & -\frac{1}{\sqrt{2}} \beta_1 k_- & 0 & \frac{1}{\sqrt{2}} \beta_1 k_- & 0 & i \gamma_1 k_+ & 0
\end{pmatrix}, \quad (18)$$

with the definitions

$$
\begin{align*}
\alpha_1 &= \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_5^e \left| \frac{\partial V}{\partial x} \right| \Gamma_1^e \right\rangle = \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_5^y \left| \frac{\partial V}{\partial y} \right| \Gamma_1^y \right\rangle, \\
\alpha_2 &= \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_5^e \left| \frac{\partial V}{\partial z} \right| \Gamma_1^e \right\rangle = \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_5^y \left| \frac{\partial V}{\partial z} \right| \Gamma_1^y \right\rangle, \\
\alpha_3 &= \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_1^e \left| \frac{\partial V}{\partial z} \right| \Gamma_1^e \right\rangle, \\
\beta_1 &= \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_5^e \left| \frac{\partial V}{\partial x} \right| \Gamma_1^e \right\rangle = \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_5^y \left| \frac{\partial V}{\partial y} \right| \Gamma_1^y \right\rangle, \\
\beta_2 &= \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_1^e \left| \frac{\partial V}{\partial z} \right| \Gamma_1^e \right\rangle, \\
\gamma_1 &= \frac{\hbar^2}{4m_0^2c^2} \left\langle \Gamma_1^e \left| \frac{\partial V}{\partial z} \right| \Gamma_1^e \right\rangle. \\
\end{align*} \quad (19)$$

Matrix representation of $H_{kp}^{(2)}$:

$$H_{kp}^{(2)} = \begin{pmatrix}
\lambda & \theta & -K^* & -H^* & 0 & 0 & 0 & 0 & T^* & 0 \\
-K & \lambda + \theta & H & 0 & 0 & 0 & T & 0 \\
-H & H^* & \lambda & 0 & 0 & U & 0 & 0 \\
0 & 0 & 0 & \lambda + \theta & -K & H & 0 & T \\
0 & 0 & 0 & -K^* & \lambda + \theta & -H & 0 & T^* \\
0 & 0 & 0 & H^* & -H & \lambda & 0 & U \\
T & T^* & U^* & 0 & 0 & 0 & V & 0 \\
0 & 0 & 0 & T^* & T & U^* & 0 & V
\end{pmatrix}, \quad (20)$$

with elements given by

$$
\begin{align*}
\lambda &= A_1 k_z^2 + A_2 (k_x^2 + k_y^2), \\
\theta &= A_3 k_z^2 + A_4 (k_x^2 + k_y^2), \\
K &= A_5 k_z^2, \\
H &= A_6 k_x k_z, \\
T &= iB_3 k_x k_z, \\
U &= i \left[ B_1 (k_x^2 + k_y^2) + B_2 k_z^2 \right] \\
V &= e_1 k_z^2 + e_2 (k_x^2 + k_y^2)
\end{align*} \quad (21)$$

and all the parameters in units of $\hbar^2 / 2m_0$.

The term $H_{kp}$ is already included in the diagonal terms of $H_{kp}^{(2)}$. Strictly speaking, the matrix representation $H_{kp}^{(2)}$ is defined as

$$H_{kp}^{(2)} = H_{kp} + \sum_{\beta} \frac{\langle \alpha | H_{kp} | \beta \rangle \langle \beta | H_{kp} | \alpha' \rangle}{E_{\alpha'} - E_{\beta}}. \quad (22)$$

The second order $k,p$ parameters $A_1$ to $A_6$ are defined the same way as Ref. [28], while $e_1$, $e_2$, $B_1$, $B_2$ and $B_3$ are given by

$$
\begin{align*}
e_1 &= 1 + \frac{2}{m_0} \sum_{\beta} \frac{\langle \Gamma_1^e | p_z | \beta \rangle^2}{E_{1e} - E_{\beta}} \\
e_2 &= 1 + \frac{2}{m_0} \sum_{\beta} \frac{\langle \Gamma_1^e | p_y | \beta \rangle^2}{E_{1e} - E_{\beta}} \\
B_1 &= \frac{2}{m_0} \sum_{\beta} \frac{\langle \Gamma_1^e | p_z | \beta \rangle \langle \beta | p_z | \Gamma_1^e \rangle}{E_{1e} - E_{\beta}} \frac{\langle \Gamma_1^e | p_z | \beta \rangle \langle \beta | p_z | \Gamma_1^e \rangle}{E_{1e} - E_{\beta}} \\
B_2 &= \frac{2}{m_0} \sum_{\beta} \frac{\langle \Gamma_1^e | p_x | \beta \rangle \langle \beta | p_x | \Gamma_1^e \rangle}{E_{1e} - E_{\beta}} \frac{\langle \Gamma_1^e | p_x | \beta \rangle \langle \beta | p_x | \Gamma_1^e \rangle}{E_{1e} - E_{\beta}} \\
B_3 &= \frac{\sqrt{2}}{m_0} \sum_{\beta} \frac{\langle \Gamma_5^e | p_z | \beta \rangle \langle \beta | p_z | \Gamma_1^e \rangle}{E_{5e1c} - E_{\beta}} \frac{\langle \Gamma_5^e | p_z | \beta \rangle \langle \beta | p_z | \Gamma_1^e \rangle}{E_{5e1c} - E_{\beta}} \\
&+ \frac{\sqrt{3}}{m_0} \sum_{\beta} \frac{\langle \Gamma_5^e | p_y | \beta \rangle \langle \beta | p_y | \Gamma_1^e \rangle}{E_{5e1c} - E_{\beta}} \frac{\langle \Gamma_5^e | p_y | \beta \rangle \langle \beta | p_y | \Gamma_1^e \rangle}{E_{5e1c} - E_{\beta}} \\
&+ \frac{\sqrt{3}}{m_0} \sum_{\beta} \frac{\langle \Gamma_5^e | p_x | \beta \rangle \langle \beta | p_x | \Gamma_1^e \rangle}{E_{5e1c} - E_{\beta}} \frac{\langle \Gamma_5^e | p_x | \beta \rangle \langle \beta | p_x | \Gamma_1^e \rangle}{E_{5e1c} - E_{\beta}}. \quad (23)
\end{align*}$$
with non-zero contributions represented by the irreducible representations in the brackets above the summation.

Appendix C: fitting in other directions

The comparison between the fitted and WIEN2k ab initio band structures is displayed in Fig. 8 for Γ-M, Γ-H and Γ-L directions. For Γ-M direction, we have the same behavior discussed for Γ-K. However, the k.p band structure in Γ-H and Γ-L directions have closer values to ab initio. This better agreement arises from the second order parameters $A_6$ and $B_3$ which only couple $k_x k_y$ plane with $k_z$, providing additional corrections to the band structures.

Figure 8: (Color online) Comparison of band structures for (a) Γ-M, (b) Γ-H and (c) Γ-L directions of InAs and (d) Γ-M, (d) Γ-H and (f) Γ-L directions of InP. The line schemes follow Fig. 4.

In Fig. 8 and Fig. 10 we show the comparison of spin splittings along Γ-M, Γ-H and Γ-L directions for InAs and InP, respectively. For Γ-H and Γ-L directions, the spin splittings are usually smaller compared to Γ-K and Γ-M. This difference, however, depends on the material and the energy band. For instance, CH and LH values for InAs in Γ-H and Γ-L are approximately half the value in Γ-K and Γ-M directions while LH and CH values for InP are approximately one fourth of the values. Because of this larger differences for InP, the spin splittings for CH bands along Γ-H and Γ-L show a small deviation compared to ab initio [Figs. 10(h) and 10(l)]. However, the crossings for HH bands [Figs. 10(f) and 10(j)] are precisely reproduced. Comparing all directions, we verify that our k.p model and parameter sets reproduce with great agreement the ab initio band structure and spin splittings along all the considered directions of the FBZ.

Figure 9: (Color online) Comparison of the InAs spin splittings for (a,e,i) CB, (b,f,j) HH, (c,g,k) CH and (d,h,l) LH along Γ-M, Γ-H and Γ-L directions, respectively. The line schemes follow Fig. 4.

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Figure 10: (Color online) Comparison of the InP spin splittings for (a,e,i) CB, (b,f,j) HH, (c,g,k) LH and (d,h,l) CH along Γ-M, Γ-H and Γ-L directions, respectively. The line schemes follow Fig. 4.

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The residue calculated for a specific direction in the FBZ is given by 
\[ r = \frac{1}{N} \sum_{n,k} \left[ f_n(\tilde{k}) - t_n(\tilde{k}) \right]^2 \],
where \( r \) runs over the 8 energy bands or 4 spin splitting curves, \( \tilde{k} \) runs over the \( k \) points, \( f_n(\tilde{k}) \) is the fitted data, \( t_n(\tilde{k}) \) is the ab initio data, and \( N \) is a normalization constant which includes the number of \( k \) points used multiplied by the size of \( n \). The total residue is the sum of the residues in all directions.
Supplemental material for the paper “Realistic multiband k.p approach from ab initio and spin-orbit coupling effects of InAs and InP in wurtzite phase”

I. CURVE FITTING FOR THE CARRIER DENSITY

In this section, we provide a curve fitting of the carrier densities presented in Figs. 7(c) and 7(d) of the main paper. The 3D parabolic model gives us a carrier density dependence of the form \( n(E) \propto E^2 \), with the proportionality constant dependent on the effective mass. Since the calculated band structures of InAs and InP do not obey this parabolic behavior, we use the functional form

\[
n(E) = a + bE + cE^d,
\]

(24)
to fit the carrier density as a function of the Fermi energy, with \( E = E_f - E_g \) for the electrons and \( E = |E_f| \) for the holes. The energy \( E \) is given in meV and the carrier density \( n \) in \( 10^{16} \text{ cm}^{-3} \). This functional form does not carry any physical meaning in its different terms, it just provides an analytical way to predict the carrier density given the Fermi energy measured from the band edge. Because of linear SOC terms in conduction band, DOS is nonzero at the energy gap, therefore the requirement to use the fitting parameter \( a \). Also, the linear dispersion \( bE \) gives a better agreement with the numerical data. For valence band, the fitting of parameters \( c \) and \( d \) is enough, and therefore \( a = b = 0 \). The best fitting is obtained by separating the carrier density in two different regions, which we call low and high energy regimes. The fitting parameters are shown in table VI.

|          | Electrons |          | Holes |
|----------|-----------|----------|-------|
| InAs low (\( E \leq 35 \)) | \( 0.0385 \) | \( 0.1115 \) | \( 0.0684 \) | \( 1.6417 \) | \( 1.1076 \) | \( 1.5923 \) |
| InAs high (\( 35 < E \leq 300 \)) | \(-9.4227 \) | \( 0.8434 \) | \( 0.0023 \) | \( 2.2664 \) | \( \) | \( \) |
| InP low (\( E \leq 35 \)) | \( 0.0117 \) | \( 0.1022 \) | \( 0.5636 \) | \( 1.5239 \) | \( \) | \( \) |
| InP high (\( 35 < E \leq 300 \)) | \(-10.1466 \) | \( 1.5372 \) | \( 0.2265 \) | \( 1.6747 \) | \( \) | \( \) |

II. ANALYTICAL DESCRIPTION FOR THE CONDUCTION BAND COMPARED TO AB INITIO

Using the analytical expressions for the conduction band provided in the main paper (section V), we show the comparison between this approach and the ab initio data in Fig. 11. Although the description for InP provides better results further away of \( \Gamma \) point, the maximum accurate energy is around 100 meV above the gap for both materials.

III. 6×6 MODEL FOR THE VALENCE BAND COMPARED TO AB INITIO

A. InAs

Applying the fitting approach discussed in Sec. IV of the main paper for the valence band of InAs, we obtain the band structure displayed in Fig. 12. In order to achieve the monotonic behavior of the valence band, i. e., decreasing energy while increasing \( k \), the resulting fitted parameters provide a band structure that is shifted to higher \( k \) values. These same trends can be seen in the spin splitting, shown in Fig. 13 by looking at the peak values. The correct fitting closer to \( \Gamma \) point does not provide the correct monotonic behavior, i. e., it either makes the spin splitting branches diverge drastically or the HH band acquires an upward curvature. Because of the small energy gap of InAs and the large SOC effects, we emphasize that including the explicit coupling with the conduction band is necessary and, therefore, the most suitable approach is the 8×8 model we discuss in the main paper.

In Fig. 14 we show the spin expectation value in \( y \) direction, \( \langle \sigma_y \rangle \), along \( \Gamma \)-K direction for InAs valence band. Despite the differences for the band structure and the spin splittings, the spin orientation follows the same trends and signs of the 8×8 model, except for the crossing in the HH band that happens for a smaller \( k \) value.
Figure 11: (Color online) Comparison between the analytical expression for conduction band and WIEN2k band structure for (a-e) InAs and (f-j) InP for Γ-(K, M, A, H, L) directions. Comparison between the analytical spin splittings for (k-n) InAs and (o-r) InP along Γ-(K, M, H, L) directions.

Figure 12: (Color online) Comparison between the 6×6 k.p model for valence band and WIEN2k band structure for InAs along (a) Γ-K, (b) Γ-M, (c) Γ-A, (d) Γ-H and (e) Γ-L.

B. InP

For InP, the fitting approach for the valence band provides a reasonable agreement for the band structure, Fig. 15, and the spin splitting, Fig. 16. It is important to note that within this 6×6 model, there is only one parameter, $A_6$, that couples $k_x(y)$ and $k_z$ wave vectors. Because InP band structure along Γ-H(L) direction is different from Γ-K(M) direction, only $A_6$ is not capable of correcting this anisotropy. Therefore, we see larger differences for the band structure and spin splittings along Γ-H and Γ-L directions.
Figure 13: (Color online) Comparison of the InAs spin splittings for (a-d) HH, (e-h) CH and (i-l) LH along Γ-(K, M, H, L) directions.

Figure 14: (Color online) Spin expectation value in $y$ direction, $\langle \sigma_y \rangle$, along Γ-K for the (a-c) $8 \times 8$ and (d-f) $6 \times 6$ model for HH, CH and LH bands. The values of $\langle \sigma_x \rangle$ and $\langle \sigma_z \rangle$ are zero along Γ-K. Solid (dashed) lines indicate the outer (inner) branch of the bands, as presented in Fig. 2(a) and 2(b) of the main paper.

In Fig. 17 we present $\langle \sigma_y \rangle$ along Γ-K direction for the valence band of InP. Although HH band in the $6 \times 6$ model shows a similar behavior, LH and CH bands do not follow the trends from the $8 \times 8$ approach. The correct description of InP spin texture, by imposing $A_7 > \alpha_1$ in the fitting process (this is seen for InAs parameters), drastically compromises the band structure and spin splittings. Therefore, we also suggest the use of $8 \times 8$ model to treat InP.
Figure 15: (Color online) Same as Fig. 12 but for InP.

Figure 16: (Color online) Same as Fig. 13 but for InP.
Figure 17: (Color online) Same as Fig. 14 but for InP.