

Edge-spin tilt and bound states in curved multiorbital graphene nanoribbons: Dominant role of d bands

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Intrinsic spin-orbit coupling (SOC) in graphene is dominated by the d orbitals, and hence, effective three orbital models with p_z and d orbitals faithfully reproduce the nontrivial band structure of the low-energy bands. However, bending and deformation are commonly described in the literature in terms of the p_z - and σ -band orbitals, owing to the assumption that the rather empty d orbitals have a marginal effect. We show in this work that the role of d orbitals is critical not only to determine spin-orbit gaps but also to account for curvature-induced spin splitting. Here we employ a multiorbital tight-binding model including the s , p , and five d orbitals of bent graphene nanoribbons with zigzag edges. We scrutinize the effects of the p or d orbitals on the intrinsic SOC splitting and on the curvature-induced Rashba-type SOC due to the onset of orbital hybridization. Whereas the former causes the edge spin to align in the direction perpendicular to the graphene plane, the latter imposes an in-plane quantization. We find that the critical curvature to observe this in-plane quantization is increased by more than 100% when the effect of the d orbitals is included, highlighting their importance. Moreover, we encounter localized bound states under sinusoidal corrugation, owing to an effective bending-induced gauge potential, which leads to a pseudomagnetic field and subsequent Landau quantization. We stress that our findings highlight the importance of d orbitals in the theoretical modeling of spintronic devices and experiments in graphene-based nanostructures.

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I. INTRODUCTION

The experimental realization of graphene almost two decades ago [1,2] modified the landscape of condensed-matter physics. Graphene exhibits a novel state of matter, the spin-Hall insulator, that is bulk insulating, yet supporting spin current via (spin-polarized) edge states [3,4]. Apart from graphene, where the detection of spin-polarized edge states is difficult due to the weak intrinsic spin-orbit coupling [5–7], synthesizing other “topological insulators” with similar properties has since been a field of active research [8]. Furthermore, methods to increase the very weak spin-orbit coupling in graphene $2d$ nanostructures and bilayer graphene via deformation [9–12] or strain [13] are actively researched.

The edge states of graphene feature a linear dispersion, and thus, perturbations due to topological defects, strain, or curvature enter as effective gauge fields [14–16]. The properties of the two-dimensional graphene electrons in gauge

fields has been extensively studied in the relation with the quantum Hall effect by using a single-orbital model [17,18]. In addition to being a playground for fundamental physics [19], gauge fields are also of interest for device applications [20–22] and may explain various phenomena in experiments of $2d$ nanostructures [23–27].

Strain-induced gauge fields allow the precise manipulation of electronic states with pseudomagnetic fields of unprecedented magnitude [28,29], which are otherwise difficult to achieve in a laboratory. The recently developed field of *strain engineering* [30,31] enables a methodology based on optoelectronics and condensed-matter physics [32–34]. However, the tight-binding models used in the explanation of these phenomena only consider the σ and p_z orbitals of carbon, where higher energy d orbitals are ignored, because the σ and p_z hybridization is expected to play a dominant role for the electronic states in bent ribbons [35]. In particular, a truncated model is commonly employed to derive the bending-induced Rashba-type spin-orbit coupling (SOC) Δ_{curv} [15,36–38]. Limitations of ignoring higher-energy bands in this case are, however, the underestimation of the intrinsic gap at the Fermi level by nearly 2 orders of magnitude, owing to the linear corrections induced by the d bands and neglecting effective Rashba-type SOC, induced by p_z - and d -orbital hybridization [4,35].

Here we employ a tight-binding model that includes up to 18 localized orbitals (s , $p_{x,y,z}$, and d_{xy,xz,yz,z^2,x^2-y^2}) with

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TABLE I. The parameters of the tight-binding model. All units are in eV.

ε_s	ε_s^H	ε_d	$V_{ss\sigma}$	$V_{ss\sigma}^H$	$V_{sp\sigma}$	$V_{sp\sigma}^H$	$V_{pp\sigma}$	$V_{pp\pi}$	$V_{pd\sigma}$	$V_{dd\sigma}$	$V_{dd\pi}$	$V_{dd\delta}$
-8.37	-2.49	12	-5.73	-6.84	5.62	7.8	8.1	3.0	3.6	3.3	-0.3	2.25

spin to describe deformed graphene nanoribbons with zigzag edges via the Slater-Koster approximation [39,40]. For circular bending perpendicular to the edges, we examine the critical curvature at which the edge spin polarization fully tilts onto the graphene plane. This is a result of the competition between intrinsic SOC Δ_I , and curvature-induced Rashba SOC, Δ_{curv} . Whereas the former results in an easy-axis edge-spin polarization, the latter demands an in-plane quantization. We compare our results for the spin-tilt obtained using 4- and 9-orbital models with results previously reported in the literature [37]. Moreover, we encounter localized bound states under sinusoidal corrugation, owing to effective bending-induced gauge potential, which leads to Landau quantization.

In Sec. II we describe the analytical model for the σ bands near the Fermi level and we extend it to include d orbitals and the SOC therein. We derive effective Rashba-type and intrinsic SOC terms, by reducing the multiorbital model to an effective p_z -orbital one. The expectation values for the spin components of the edges states are used to discuss the spin alignment of the edge states in bent ribbons. In Sec. III we focus on the effect of deformation-induced gauge fields and summarize our work in Sec. IV.

II. TIGHT-BINDING MODEL AND PARAMETRIZATION

The formalism is adapted from [41,42], where the downfolding of a multiorbital tight-binding Hamiltonian in flat graphene is described and used for analyzing the hopping paths of an electron between different orbitals. A deformation breaks the symmetry along the normal plane and thus changes the hopping matrix elements. This causes hybridization with formerly symmetry-forbidden orbitals, allowing Rashba SOC terms. In order to understand the occurrence of the bending-induced SOC terms, we employ an effective next-nearest-neighbor (NNN) Löwdin transformation, allowing one to identify the contributing terms.

A. Graphene nanoribbons passivated with hydrogen atoms

In flat graphene nanoribbons with zigzag edges, the regular sp^2 hybridization of the graphene lattice is modified at the edges. In the low-energy approximation the dominant bulk contribution stems from the p_z orbitals, with the well-known linear dispersive Dirac cones and low-dispersing edge states. As graphene is bent, however, the dangling bonds located at the edges where the sp^2 hybridization breaks couple to the p_z orbitals, modifying in turn the dispersion of the edge states. We include the passivation of the edge sites with hydrogen atoms in the model explicitly for all of the numerical calculations in the following.

At the hydrogen sites, as depicted in Fig. 1(a), we employ only localized hydrogen s orbitals, which couple to the four s and p orbitals of the neighboring carbon (white circles).

The parameters for all the Hamiltonians, including the hydrogen, s , p , and d orbitals used later are given in Table I, where we employ the commonly used Slater-Koster couplings, with an energy shift relative to the p orbitals of graphene of ε_s^H [37], whereas the s orbitals of graphene are at ε_s [35].

We describe the atomic dislocation via $h(y)$ as illustrated for constant curvature in Fig. 1(b) and for sinusoidal bending along the arrow depicted in (c). As a consequence of the deformation, the edge spins [purple and green in Fig. 1(b)] tilt into the graphene plane, whereas for flat graphene these are normal to the surface.

B. Atomistic SOC

As has been established theoretically [41] and experimentally [43], intrinsic SOC in flat graphene is dominated by the d orbitals. However, in the presence of bending, the p orbitals hybridize, allowing for Rashba-type SOC. We thus consider both the p and the d orbitals in our calculation. Here, we express the cartesian atomic p_x , p_y , and p_z orbitals via the complex spherical harmonics [44], where the SOC reads

$$H_{\text{SOC}}^p = \xi_p^0 \begin{pmatrix} 0 & -i\hat{s}^z & i\hat{s}^y \\ i\hat{s}^z & 0 & -i\hat{s}^x \\ -i\hat{s}^y & i\hat{s}^x & 0 \end{pmatrix}, \quad (1)$$

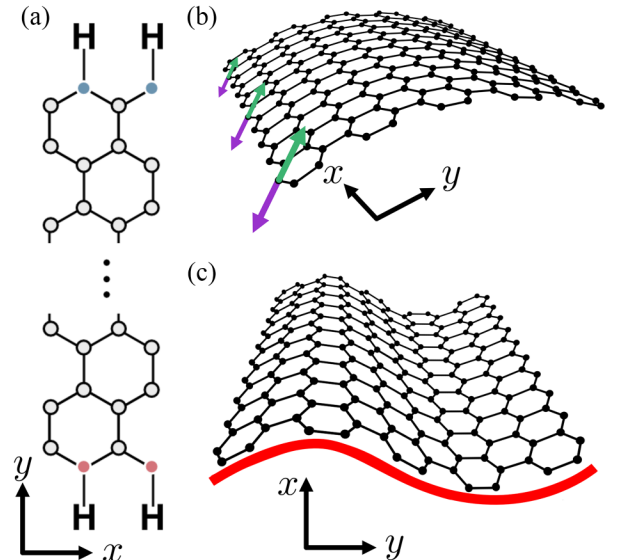


FIG. 1. (a) A graphene nanoribbon with periodic boundary conditions along the horizontal x direction with zigzag edges, passivated by hydrogen atoms along the y direction. The white circles represent carbon atoms and the red and blue colors denote edge sites. (b) Circular bending along the y direction perpendicular to the zigzag edges. The tilted edge state spins, given by the expectation value of the spin components, are shown in purple and green. (c) Sinusoidal bending along the y direction, denoted by the red line.

where $\hat{s}^j$ are the Pauli matrices. In the basis of directed d orbitals $\{d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{z^2}\}$, the atomistic SOC operator for the d orbitals becomes

$$H_{\text{SOC}}^D = \xi_d^0 \begin{pmatrix} 0 & 2i\hat{s}^z & -i\hat{s}^x & i\hat{s}^y & 0 \\ -2i\hat{s}^z & 0 & i\hat{s}^y & i\hat{s}^x & 0 \\ i\hat{s}^x & -i\hat{s}^y & 0 & -i\hat{s}^z & i\sqrt{3}\hat{s}^y \\ -i\hat{s}^y & -i\hat{s}^x & i\hat{s}^z & 0 & -i\sqrt{3}\hat{s}^x \\ 0 & 0 & -i\sqrt{3}\hat{s}^y & i\sqrt{3}\hat{s}^x & 0 \end{pmatrix}. \quad (2)$$

We employ here the intrinsic SOC parameters $\xi_p^0 = 5$ meV [37] and $\xi_d^0 = 0.8$ meV [35].

C. 4-orbital model with σ bands

For the sake of simplicity, we start with a four-orbital model, which will be straightforwardly extended in the following sections. We employ a tight-binding Hamiltonian [42] in order to describe a nanoribbon as depicted in Fig. 1(a) with the formalism of a previous work on this topic [35] where the atomistic SOC is defined as (1):

$$\hat{H}_P = \sum_{\langle i,j \rangle} t_{\alpha'\beta'}^{ij} \hat{c}_i^{\dagger\alpha'} \hat{c}_j^{\beta'} - i\xi_p^0 \varepsilon_{\alpha\beta\gamma} \hat{s}^\alpha \hat{c}_i^{\dagger\beta} \hat{c}_i^\gamma. \quad (3)$$

Here $\hat{c}_i^{(\dagger)\alpha}$ are the annihilation (creation) operators at site i and orbitals $\alpha', \beta' \in \{s, x, y, z\}$, while $\alpha, \beta, \gamma \in \{x, y, z\}$. The hydrogen sites denoting passivation at an edge are included explicitly with the first term of Eq. (3), whenever i and j denote one carbon edge site and one hydrogen site each. $\langle \cdot \rangle$ denotes nearest neighbors (NNs), $\varepsilon_{\alpha\beta\gamma}$ is the completely antisymmetric Levi-Civita tensor, and the Einstein summation convention is assumed. Bending and deformation are described in terms of matrix element, $t_{\alpha'\beta'}^{ij}$. To this end, we first define the *local* quantization axes, which are described in terms of NN-relative angles θ . Together with the bond angle ψ these angles encode the bending strength and local curvature of the deformation, as illustrated in Fig. 2(a). The corresponding matrix elements are listed in Appendix C.

We derive in Appendix A an effective NNN model for the p_z orbitals. We use the shorthand notation $t_{\alpha,\beta}(\theta_n) := t_{\alpha,\beta}^{0n}$, where $t_{\alpha,\beta}(\theta_{n'}) := t_{\alpha,\beta}^{nn'}$, to emphasize the local bending strength at each site. The NN and NNN of each site are shown in Fig. 2(b).

We classify the different corrections as A , B , and C . The A terms are spin independent, whereas the B yields a spin splitting and the C term opens a spin-orbital gap. The former is a result of the bending-induced spin-orbit coupling, whereas the latter is nonzero in flat graphene, commonly termed as intrinsic spin-orbit coupling. Thus, the NNN hopping model for the wave-function coefficients $a_{\alpha,0}$ takes the following form:

$$(\varepsilon - \varepsilon_p - \varepsilon'')a_{z,0} = A_n + A_{nn} + B_{nn} + C_{nn}, \quad (4)$$

where ε'' is the energy renormalization due to the hybridization of p_z and σ orbitals. The index n denotes hopping terms between site 0 to neighboring sites, while nn labels NNNs hopping.

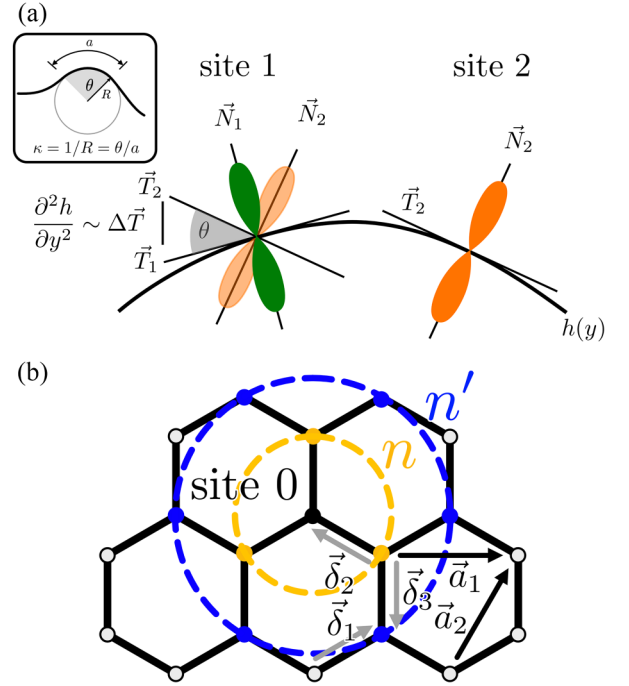


FIG. 2. (a) Localized p_z orbitals at sites 1 and 2, where the relative angle $\theta \sim \frac{\partial^2 h}{\partial y^2}$ is given by the tangential vectors $\vec{T}_{1/2}$ and normal vectors $\vec{N}_{1/2}$ for a deformation $h(y)$. The inset shows the relation of curvature κ and local bending radius R . (b) Plaqueette and displacement vectors of the graphene lattice, $\vec{\delta}_1 = \frac{a}{2}(\sqrt{3}, 1)$, $\vec{\delta}_2 = \frac{a}{2}(-\sqrt{3}, 1)$, and $\vec{\delta}_3 = -a(1, 0)$. In the definition of the tight-binding model the nearest neighbors of a site 0 are denoted n and its next-nearest neighbors n' .

As we will see below, the spin alignment can be described in terms of a competition of these relative spin-orbit coupling terms. While curvature-induced strain, such as for carbon nanotubes, leads to an overall energy shift [45], we focus here on effects that modify the spin splitting, originating from curvature-induced SOC.

The hopping paths for the different terms are given in Fig. 3 and the order of the processes and their spin dependence is shown in Table II. NN hopping together with a spin-flip term (labeled “ n ”) yield no net spin splitting, owing to

TABLE II. The order of each of the processes in either hopping parameters or spin-orbit coupling parameters. For the SOC terms, the proportionality to the spin operators is also listed.

	Hopping	Δ_{SOC}
A_n	$\sim t_{z,z}(\theta_n)$	
A_{nn}	$\sim t_{z,x}(\theta_n)t_{x,z}(\theta_{n'})$	
B_{nn}	$\sim t_{z,s}(\theta_n)t_{s,x}(\theta_{n'})$	$\sim \xi_p^0 \hat{s}^x/y$
C_{nn}	$\sim t_{x,s}(\theta_n)t_{s,y}(\theta_{n'})$	$\sim (\xi_p^0)^2 \hat{s}^z$
A_{nn}^D	$\sim t_{z,xz}(\theta_n)t_{xz,z}(\theta_{n'})$	
$B_{nn}^{D,1}$	$\sim t_{x,xz}(\theta_n)t_{xz,z}(\theta_{n'})$	$\sim \xi_p^2 \hat{s}^x/y$
$B_{nn}^{D,2}$	$\sim t_{z,yz}(\theta_n)t_{xy,z}(\theta_{n'})$	$\sim \xi_d^2 \hat{s}^x/y$
C_{nn}^D	$\sim t_{z,yz}(\theta_n)t_{xz,z}(\theta_{n'})$	$\sim \xi_d \hat{s}^z$

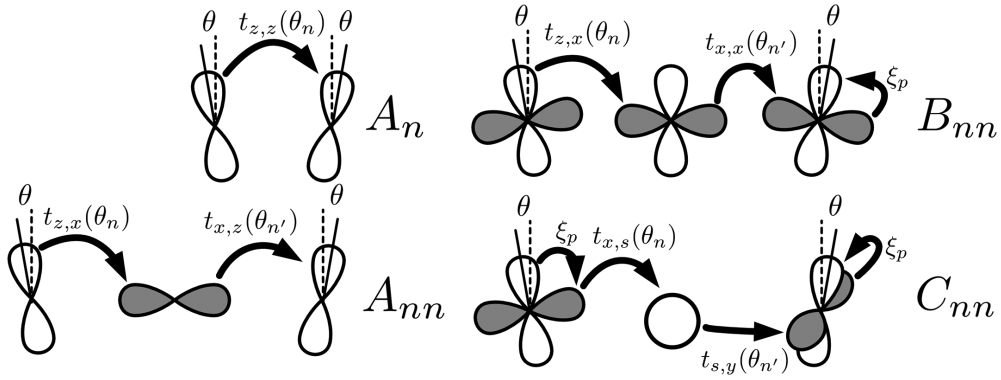


FIG. 3. Hopping paths for the different terms in the four-orbital model. The terms with index n denote nearest-neighbor and those with nn denote next-nearest-neighbor hopping. In order to distinguish p_x and p_y from p_z orbitals at a site, gray shading is used.

time-reversal symmetry. Indeed the first correction appears at second order in hopping (labeled “ nn ”) and first order in SOC, as we will see.

The NN and second NN hopping terms A_n and A_{nn} are given in Appendix A 2 and shown in Fig. 3, but do not play an important role in the spin splittings, and hence, we leave these out of our discussion. B_{nn} and C_{nn} denote the Rashba-type SOC Δ_{curv} and the intrinsic SOC Δ_I , respectively, and their most dominant contributions are given by

$$B_{nn} = i \frac{\xi_p^0}{\varepsilon_\sigma \varepsilon_s} \sum_{n,n' \neq 0} (\hat{s}_y [t_{z,s}(\theta_n) t_{s,x}(\theta_{n'}) - t_{x,s}(\theta_n) t_{s,z}(\theta_{n'})] - \hat{s}^x [t_{z,s}(\theta_n) t_{sy}(\theta_{n'}) - t_{y,s}(\theta_n) t_{sz}(\theta_{n'})]) a_{z,n'}, \quad (5)$$

$$C_{nn} = - \frac{i(\xi_p^0)^2 \hat{s}^z}{\varepsilon_\sigma^2 \varepsilon_s} \sum_{n,n' \neq 0} [t_{x,s}(\theta_n) t_{s,y}(\theta_{n'}) - t_{y,s}(\theta_n) t_{s,x}(\theta_{n'})] a_{z,n'}, \quad (6)$$

which are also shown in Fig. 3. B_{nn} describes hopping from p_z to a neighboring σ orbital, followed by another hopping to a next-nearest-neighbor σ orbital, together with an on-site (SOC) spin flip. Hence, this term is linear in SOC ξ_p^0 and quadratic in hopping. B_{nn} yields a bending-induced splitting and an in-plane spin alignment [37]. This term vanishes in flat graphene due to symmetry. In contrast C_{nn} arises from an on-site spin flip provided by SOC within the σ band, hopping to a NNN therein, and an on-site spin flip back to a p_z orbital, yielding a second-order correction in SOC, that is, quadratic in ξ_p^0 .

In view of these dominant processes with different quantization directions, we proceed to quantify and define the *spin alignment*. The normal vector at an edge site l is given by $\vec{v} = \vec{v}_1 \times \vec{v}_2$, where $\vec{v}_1$ and $\vec{v}_2$ are unitary vectors pointing from site l to two NNs [see Fig. 2(b)]. The alignment of the spin operator expectation value

$$\langle \hat{s}_i(l) \rangle = \sum_{\sigma\sigma'} \sum_{\mu\nu} a_{l\mu\sigma}^\dagger a_{l\nu\sigma'} \hat{s}_i^{\sigma\sigma'} \quad (7)$$

with respect to the local normal at the sample edges defines the tilting angle

$$\cos \varphi_{p/d} = \frac{\vec{v} \cdot \langle \hat{s} \rangle}{|\vec{v}| \cdot |\langle \hat{s} \rangle|} \quad (8)$$

at site l .

For small deformations as depicted in Fig. 1(b), we consider the alignment angle φ_p as a result of the competition between the intrinsic SOC and curvature-induced SOC. Thus, the spin alignment is approximately given by

$$\varphi_p \sim \frac{\Delta_I}{\Delta_{\text{curv}}} \sim \frac{|C_{nn}(\theta)|}{|B_{nn}(\theta)|} \sim \frac{1}{|\varepsilon_\sigma|} \frac{\xi_p^0}{\theta}. \quad (9)$$

A quantity of interest is the critical bending radius R_c at which the spin of the edge states becomes parallel to the graphene plane, that is, they tilt to $\varphi = \pi/2$. Since $\theta \sim 1/R$, we obtain

$$\frac{1}{R_c} \sim \xi_p. \quad (10)$$

D. 9-orbital model

The effective hopping for the p_z orbitals with 9 orbitals is obtained by a similar procedure as the previous model for four orbitals in Sec. II C, and detailed in the Appendix A. The Hamiltonian (3) with additional d orbitals is given by

$$\hat{H}_D = \sum_{(i,j)} t_{\delta,\delta'}^{ij} \hat{c}_i^{\dagger\delta} \hat{c}_j^{\delta'} + \Lambda_\alpha^\beta \hat{c}_i^{\dagger\alpha} \hat{c}_i^\beta + \Upsilon_\mu^\nu \hat{c}_i^{\dagger\mu} \hat{c}_i^\nu. \quad (11)$$

As before $\alpha, \beta \in \{x, y, z\}$, while $\delta, \delta' \in \{s, x, y, z, xy, xz, yz, z^2, x^2 - y^2\}$ and $\mu, \nu \in \{xy, xz, yz, z^2, x^2 - y^2\}$. The SOC is given by (1) and (2) and denoted by Λ_α^β and Υ_μ^ν , respectively. The hydrogen passivation is included only in the first part of the Hamiltonian (11). Application of the same derivation of a NNN hopping model as before leads to

$$(\varepsilon - \varepsilon_p - \varepsilon'' - \varepsilon_d'') a_{z,0} = A_n + A_{nn} + B_{nn} + C_{nn} + A_{nn}^D + B_{nn}^D + C_{nn}^D, \quad (12)$$

where the dominant contributions of the additional d -orbital terms are given by

$$B_{nn}^D = B_{nn}^{D,1} + B_{nn}^{D,2} = \frac{i\xi_p^0}{\varepsilon_\sigma \varepsilon_d} \sum_{n,n' \neq 0} \{ \hat{s}_y [t_{x,xz}(\theta_n) t_{xz,z}(\theta_{n'}) + t_{x,yz}(\theta_n) t_{yz,z}(\theta_{n'})] - \hat{s}_x [t_{y,xz}(\theta_n) t_{xz,z}(\theta_{n'}) + t_{y,yz}(\theta_n) t_{yz,z}(\theta_{n'})] \} a_{z,n'}$$

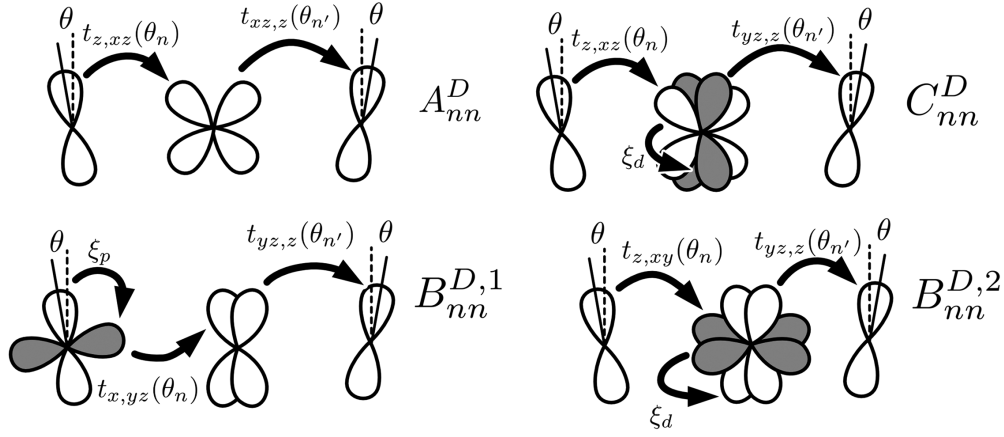


FIG. 4. Hopping paths for the different terms in the 9-orbital model. The terms are denoted with superscript D and those with index n denote nearest-neighbor and those with nn denote next-nearest-neighbor hopping. In order to distinguish p_x and p_y from p_z orbitals and d_{yz} from d_{xy} and d_{xz} orbitals at a site, gray shading is used.

$$+ \frac{i\xi_d^0}{\varepsilon_d^2} \sum_{n,n' \neq 0} [\hat{s}_y[t_{z,yz}(\theta_n)t_{xy,z}(\theta_{n'}) - t_{z,xy}(\theta_n)t_{yz,z}(\theta_{n'})] \\ - \hat{s}_x[t_{z,xy}(\theta_n)t_{xz,z}(\theta_{n'}) - t_{z,xz}(\theta_n)t_{xy,z}(\theta_{n'})]a_{z,n'}, \quad (13)$$

$$C_{nn}^D = \frac{i\xi_d^0 \hat{s}_z}{\varepsilon_d^2} \sum_{n,n' \neq 0} [t_{z,yz}(\theta_n)t_{xz,z}(\theta_{n'}) - t_{z,xz}(\theta_n)t_{yz,z}(\theta_{n'})]a_{z,n'}, \quad (14)$$

and the order of each term in both hopping and SOC is given in Table II. The term A_{nn}^D denotes the direct hopping between NNN, but unlike the term A_{nn} introduced above, the process involves an intermediate d orbital. The matrix elements $t_{z,xz}(\theta_n)$ and $t_{z,yz}(\theta_n)$ are the dominant contributions. The bending-induced SOC B_{nn}^D is comprised of a term with p -orbital SOC and another with d -orbital SOC (see Fig. 4). C_{nn}^D has the role of intrinsic SOC and scales linearly with ξ_d^0 . Recall that C_{nn} scales quadratically with ξ_p^0 in the 4-orbital model. In fact, the analog of Eq. (9) for the 9-orbital model yields

$$\varphi_d \sim \frac{\Delta_I}{\Delta_{\text{curv}}} \sim \frac{|C_{nn} + C_{nn}^D|}{|B_{nn} + B_{nn}^{D,1} + B_{nn}^{D,2}|}(\xi_p, \xi_d) \\ \sim \left(\frac{a_0 \xi_p^2}{a_1 \xi_p + a_2 \xi_d} + \frac{b_0 \xi_d}{a_1 \xi_p + a_2 \xi_d} \right) \frac{1}{\theta}, \quad (15)$$

where a_0 , a_1 , a_2 , and b_0 contain $V_{pd\pi}$, $V_{pd\sigma}$, $V_{sp\sigma}$, and ε (15). Since $|C_{nn}| < |C_{nn}^D|$ and $a_2 \ll a_1$, fixing $\xi_d = \xi_d^0$ we find the dependency with ξ_p :

$$\varphi_d \sim \left(\frac{a_0}{a_1} \xi_p + \frac{1}{\frac{a_1}{b_0 \xi_d^0} \xi_p + \frac{a_2}{b_0}} \right) \frac{1}{\theta}, \quad (16)$$

yielding a different functional for the critical curvature,

$$\frac{1}{R^c(\xi_p)} \sim \frac{1}{\xi_p}. \quad (17)$$

However, fixing $\xi_p = \xi_p^0$, we obtain

$$\frac{1}{R^c(\xi_d)} \sim \xi_d. \quad (18)$$

A comprehensive analytical model is developed in Appendix B, where the critical curvature is derived within a perturbative approach, where ξ_p and ξ_d are the small parameters. The analytical expression is then employed to fit the numerical data [solid lines of Fig. 5(b)].

The impact of the d orbitals is illustrated in Fig. 5(a), where the spin alignment of the edge states of a 56-C atom nanoribbon is represented as a function of the curvature $\kappa = 1/R$, as illustrated in Fig. 2. Within a 4-band model (dashed lines) we obtain a critical curvature of $1/R^c \approx 0.018 \text{ nm}^{-1}$, close to the result obtained by Gosálbez-Martínez *et al.* [37]. However, the nine-band model (solid lines), a critical

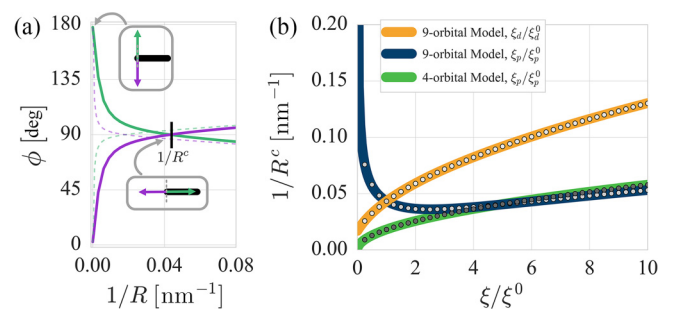


FIG. 5. (a) Tilt angle of spin with the local surface normal of the Kramers pair that form the edge states (purple and green curves) as a function of the curvature R^{-1} , evaluated at $k_x a = 10^{-2}$. The ribbon has 56 C atoms and is computed with the nine-orbital model (solid) and the four-orbital model (dashed). A point is marked $1/R^c$, where both spins align at 90° with respect to the surface normal. The insets show a side view (in the yz plane) of the ribbon (black) and the relative orientation of the edge state spins to the local surface normal (dashed). (b) Dependence of the critical bending radius $1/R^c$ as a function of the dimensionless SOC parameter when the p - and d -orbital SOC strength is varied for the 4- and 9-orbital model in units of $\xi_p^0 = 5 \text{ meV}$ and $\xi_d^0 = 0.8 \text{ meV}$. The dots correspond to a fit, which is discussed in Appendix B.

curvature of $1/R^c \approx 0.043 \text{ nm}^{-1}$ is obtained, which is more than double the previous result, highlighting the importance of the d orbitals for describing strain-related phenomena.

Figure 5(b) shows the critical curvature as a function of the p - and d -orbital SOC parameters relative to the established parameters ξ_p^0 and ξ_d^0 , respectively. The 4-orbital model yields a critical curvature that monotonically increases with ξ_p , as expected from (10) [green in Fig. 5(b)]. However, the picture changes when the d orbitals are included (blue): These orbitals trend to align the spin in the out-of-plane direction, resulting in a competing effect. Hence, for $\xi_p \ll \xi_{p,d}^0$, a large curvature is required to tilt the spin, whereas the 4-band model trend is recovered for $\xi_p/\xi_p^0 \gtrsim 2$, where the effect of the d orbitals becomes negligible.

Considering the full model with d orbitals in Fig. 5(b) shows also that the critical curvature increases with ξ_d , in agreement with (18), highlighting the relevance of the d orbitals. A more thorough analysis of these terms is done in Appendix B via a fit to the numerical data.

III. LANDAU LEVELS AND BOUND STATES

In general, strain in Dirac materials leads to gauge fields, as the deformation modifies the hopping or, equivalently, the Fermi velocity [1]. To illustrate the effect of these gauge fields and the origin of Landau quantization in the dominant p_z bands, we employ an effective one-orbital tight-binding model [35,46,47], allowing us to describe the angular dependency of $t_{\alpha',\beta'}^{ij}$ in Eq. (3) perturbatively. The one-orbital Fourier transformed (FT) Hamiltonian now reads

$$H_{\mathbf{k}} = \sum_{i=1}^3 [t + \delta t(\mathbf{r}, \delta_i)] e^{-i\delta_i \mathbf{k}} \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} + \text{H.c.}, \quad (19)$$

where $t = t_{p_z,p_z}^{i,i+1}$, δ_i is the unit vector along the bond direction, and $\hat{\alpha}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}}$ the FT annihilation and creation operators at sublattices A and B , respectively. The anisotropic deformation is perturbatively included in $\delta t(\mathbf{r}, \delta_i)$. Note that SOC is left out for simplicity. Within the low-energy approximation in the vicinity of the Dirac points $\vec{K} = (\tau \frac{4\pi}{3\sqrt{3}a}, 0) + (q_x, q_y)$, for $|\vec{q}| \ll |\vec{K}|$ with $\tau = \pm 1$ selecting the valley, we obtain the modified well-known Dirac Hamiltonian,

$$H_{\mathbf{k}} = v_F \hbar [(\tau \hat{\sigma}_x q_x + \tau A_x) + \hat{\sigma}_y (q_y + \tau A_y)], \quad (20)$$

where $v_F = -\frac{3\tau a}{2\hbar} \approx 10^6 \text{ m/s}$ is the Fermi velocity [1] and a the lattice constant. Here, $\hat{\sigma}_z = \pm 1$ describes the sublattice spin, with $\hat{\sigma}_i$ being the usual Pauli matrices. Including bending perturbatively, the pseudovector potential $\vec{A} = (A_x, A_y)$ arises naturally [16], where we have defined

$$\begin{aligned} \hbar v_F A_x &= \delta t(\mathbf{r}, \delta_3) - \frac{1}{2} [\delta t(\mathbf{r}, \delta_1) + \delta t(\mathbf{r}, \delta_2)], \\ \hbar v_F A_y &= -\frac{\sqrt{3}}{2} [\delta t(\mathbf{r}, \delta_2) - \delta t(\mathbf{r}, \delta_1)]. \end{aligned} \quad (21)$$

For a sinusoidal bending along y [i.e., perpendicular to the zigzag edge; see Fig. 1(c)], it is easy to see that $\delta t(y, \delta_1) = \delta t(y, \delta_2) \simeq 0$.

Minimal substitution within the Slater-Koster approximation leads to an explicit pseudopotential and a local pseudomagnetic field, $\mathbf{B} = \nabla \times \mathbf{A}$:

$$A_x = \frac{a}{3} \left(\frac{V_{pp\sigma}}{V_{pp\pi}} - 1 \right) \kappa^2(y), \quad A_y = 0, \quad (22)$$

$$B_z(y) = -\frac{a}{3} \left(1 - \frac{V_{pp\sigma}}{V_{pp\pi}} \right) \kappa(y) \frac{\partial \kappa(y)}{\partial y}, \quad (23)$$

where we used $\sin \theta \approx \frac{a}{R}$ and we employed for the curvature terms of the bending profile $h(y)$ [48]

$$\kappa = \frac{1}{R} = \frac{h''}{[1 + (h')^2]^{3/2}} \quad (24)$$

[see Fig. 2(a)]. For our sinusoidal bending $h(y) = h_0 \sin(\frac{2\pi}{\lambda} y)$. In the soft corrugation limit, $h_0 \ll \lambda$, we have

$$A_x(y) = \frac{\sin^2 2\pi y/\lambda}{l_a}, \quad B_z(y) = -\frac{2\pi}{\lambda l_a} \sin(4\pi y/\lambda), \quad (25)$$

where we have defined for convenience the length

$$l_a = \frac{1}{V_{pp\sigma}/V_{pp\pi} - 1} \left(\frac{\lambda}{2\pi} \right)^4 \frac{3}{ah_0^2}. \quad (26)$$

Periodic translations along x allow us to employ the usual ansatz, $\psi^{A/B}(x, y) = e^{ik_x x} f^{A/B}(y)$. Solving the Schrödinger equation for both sublattice components yields

$$[\hbar v_F (\tau k_x + A_x(y) - \hat{\partial}_y)] f^A(y) = E_A f^A(y), \quad (27)$$

$$[\hbar v_F (\tau k_x + A_x(y) + \hat{\partial}_y)] f^B(y) = E_B f^B(y), \quad (28)$$

where we have defined $\hat{p}_y \equiv -i\hat{\partial}_y$. We now focus on the regions where the magnetic field is strongest and $\mathbf{A}$ is linear, that is, at $y \simeq \lambda/8$. Substituting the expression for $f^A(y)$ from Eq. (28) into Eq. (27), we obtain the harmonic oscillator (HO), resulting in potential Landau levels:

$$\frac{1}{2m} [\hbar^2 B_z^2 (y - y_0)^2 + \hat{p}_y^2] f^B = \frac{(E^2 + \hbar^2 v_F^2 B_z^2)}{2m v_F^2} f^B,$$

where m is introduced for convenience, allowing one to identify the Dirac frequency, $\omega_D = \hbar B_z/m$. The eigenvalues are then given by $\hbar \omega_D (2n + 1) = (E^2 + \hbar^2 v_F^2 B_z^2)/m v_F^2$, and the eigenfunctions are HOs centered at $y_0 = \tau k_x l_B^2$, where $l_B = 1/\sqrt{|B_z|} \propto \sqrt{l_a \lambda}$ is a characteristic length scale that governs any quantum phenomena in a pseudomagnetic field: These eigenfunctions consist of stripes, extended along the x direction and exponentially localized around y_0 within a distance given by l_B . For the nanoribbon considered here, $\lambda \sim 15a$, $V_{pp\pi} \sim -3 \text{ eV}$, $V_{pp\sigma} \sim 6 \text{ eV}$, and $v_F \sim 3 \times 10^6 \text{ m/s}$, we obtain $l_B \sim 1 \text{ nm}$, which is reasonable. We consider now the numerical results, first employing the 4-orbital model including the passivation via hydrogen atoms. Figure 6(a) shows the band structure of sinusoidally bent graphene with two solutions highlighted (green and purple). If passivation with the hydrogen atoms at the edges was not included, the sp^2 hybridization would be perturbed locally, reducing the slope of the dispersion relation of the edge

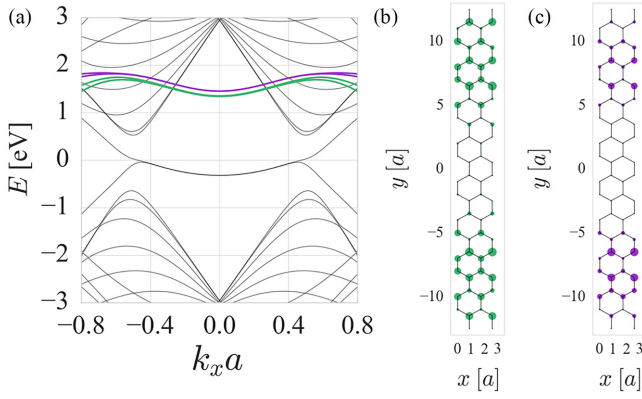


FIG. 6. (a) Band structure of a sinusoidally bent nanoribbon using the 4-orbital model. The colored bands (green, purple) appear due to the pseudomagnetic field and represent localized states, shown in (b) and (c) with their respective color, evaluated at $k_x a = 0.16$. The dot size is proportional to the corresponding occupation of a lattice site.

states in Fig. 6(a) around $k_x = 0$. Furthermore additional states with flat dispersion, shifted by several eV below could be observed. However, these states are not relevant for the

bending-induced localized states for our discussion and will no longer be regarded. The spatial distribution of these two solutions evaluated at $k_x a = 0.16$ is shown in Figs. 6(b) and 6(c) matching the color code of Fig. 6(a). The deformation is characterized by $\lambda = 15a$ and $h_0 = 2.9a$.

Next We perform the numerical computation employing a 9-orbital model with spin. The hybridization of the p and d orbitals yields a higher localization, especially close to where the curvature of the deformation is maximal, as Fig. 7(a) shows. The pseudomagnetic field and vector potential are shown in Fig. 7(b), where the round and square points are numerical results computed from the matrix elements $t_{zz}[\theta(y)]$ of the bent and flat ribbon t_{zz} for each of the bonds, using Eq. (21).

The analytical results are computed using the full curvature expression in Eq. (24) using Eq. (22) and in Eq. (23), respectively, and are shown as solid lines. The discrepancy of the numerical and analytical results originates from the stiff bonds of the graphene ribbons used in the numerical computation as compared to the differentiable curvature, employed in the analytical formula. Figure 7(c) shows the local weight of the solutions of (a) with the same color coding. We observe that the localization is larger at those points where $|A|$ is more

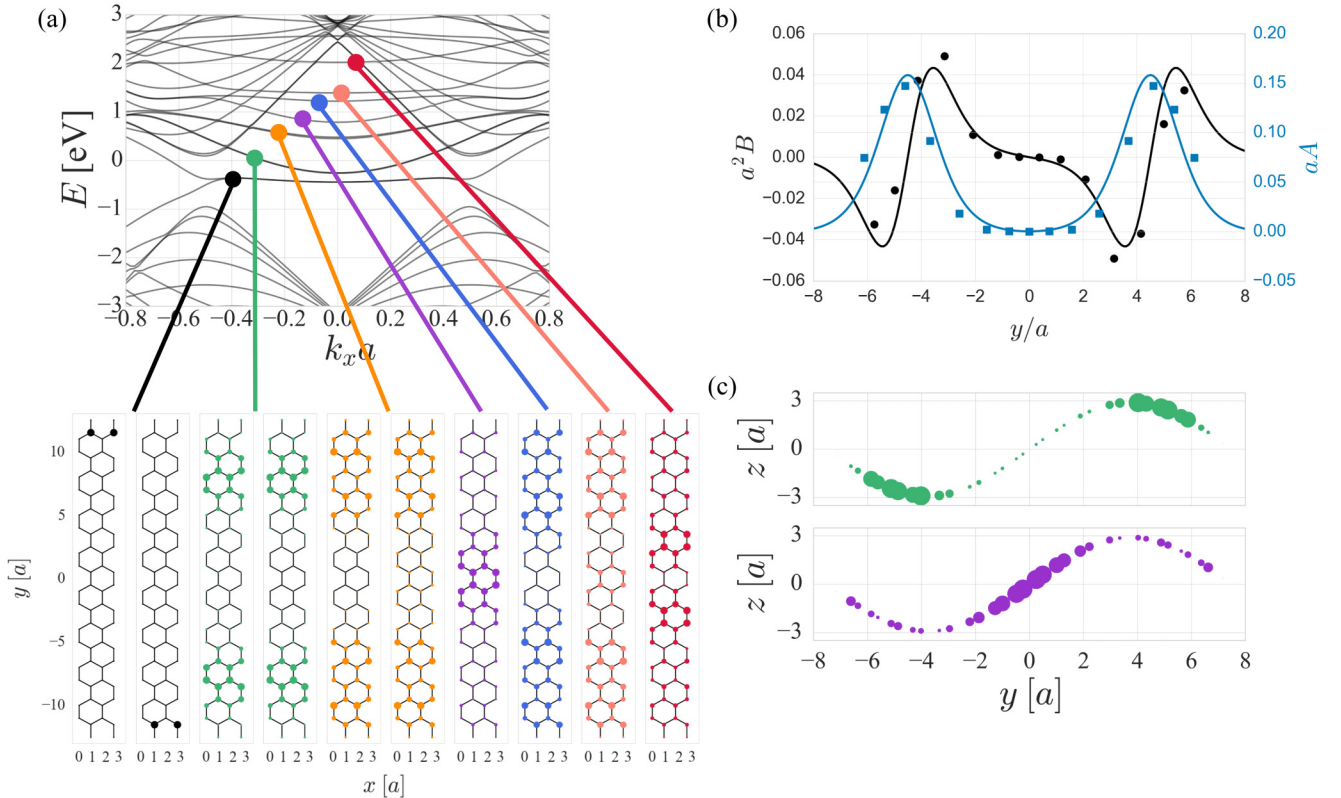


FIG. 7. (a) Dispersion relation (top) of a deformed nanoribbon with 16 rows and sinusoidal deformation with amplitude $2.9a$ and wavelength $15a$ for the 9-orbital model. The different localized states are computed at $k_x a = 1.6 \times 10^{-2}$ and are indicated by color (bottom). (b) Pseudomagnetic field B and pseudovector potential A as a function of the y coordinate obtained from numerical computation of the tight-binding model (circles and squares) and theoretical curve (solid lines). (c) Side view of the deformation and the spatial occupation of the green and purple states from (a), evaluated at $k_x a = 1.6 \times 10^{-2}$. The axes are aligned with (b) to highlight that the states localize around points where the pseudomagnetic field switches sign. Note that the coordinate axes in (a), (b), and (c) show the same ribbon, but in (a) the vertical y -axis range is parametrized by the coordinates of the unbent ribbon, while in (b) and (c) in the side view along the ribbon the vertical z -axis deformation $h(y)$ leads to a rescaling of the horizontal y -axis range.

prominent (larger curvature κ), with the lowest state (green) occurring at $y \sim \lambda/8$ and $y \sim 7\lambda/8$.

IV. CONCLUSION

We have investigated the effect of the d orbitals on the spin alignment of the gap crossing edge states in deformed single layer graphene, as well as the occurrence of bending-induced localized states in the bulk. Bending of graphene nanoribbons induces an effective Rashba-type SOC, as a consequence of the broken symmetry along the surface normal, which causes an in-plane alignment of the edge state spins. This effective term occurs due to the hybridization of the p_z - and sp^2 -hybridized orbitals. A 4-orbital model reveals that an increased atomistic SOC leads to a tendency for aligning the edge's spins parallel to the (local) out-of-plane direction, counteracting the tendency for in-plane alignment of the edge state spins due to the bending.

By employing a 9-orbital model other Rashba-type mechanisms arise due to the hybridization of p and d orbitals. Our numerical computations reveal a stiff spin direction, that is, a higher curvature is needed for an in-plane alignment when the d orbitals are included in the calculation.

We expect our results to be applicable to other materials with hexagonal lattices, such as germanene and silicene, as well. Effective hopping paths such as in our analysis, however, will compete with the existing hybridization, where the intrinsic SOC is not relevant [49], due to out-of-plane sites in such lattices. We expect that the impact of bending will likely be diminished and so will be the implications of our analysis. For deformed graphene nanoribbons on the other hand, in addition to the onset of bending-induced SOC, the hybridization with d orbitals results in an increased sensitivity to strain, resulting in additional Landau levels in pseudomagnetic fields that localize near points of maximal curvature. This highlights the importance of the d bands, which are required for a correct description of the SOC splitting, the spin alignment, and the strain-induced Landau levels. These results should stimulate future spintronic-based theoretical and experimental work on graphene-based nanostructures, where the effect of the d orbitals, even if barely populated, should not be disregarded. In particular, spin tilt would yield information on the Rashba to intrinsic SOC ratio, which could be measured employing electron spin resonance [50] or spin-polarized scanning tunneling microscopy [5].

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: THE NNN HOPPING MODEL

1. Derivation of the NNN hopping model 4-orbital model

We seek an analytical solution of Eq. (3) in the bulk using a common ansatz for the wave function [35]. Because

the functional dependency will be identical for hopping to a neighboring hydrogen site instead of the carbon sites close to the edges of the sample, this case will not be considered for the analytical results in the following. We first choose a reference site “0,” with wave-function coefficients $a_{\alpha,0}$, where the spin index σ is omitted for brevity. Likewise, the coefficients of the three adjacent sites are given by $a_{\alpha,n}$, where $n \in \{1, 2, 3\}$ and θ_n is their relative angle. We label the NNN coefficients as $a_{\alpha,n'}$, with $\theta_{n'}$ being the angle between sites n and n' [see Fig. 2(b)]. We obtain the secular equations for the s and p orbitals, respectively:

$$(\varepsilon - \varepsilon_s)a_{s,0} = \sum_n t_{s,s}a_{s,n} + \sum_{\alpha,n} t_{s,\alpha}(\theta_n)a_{\alpha,n}, \quad (\text{A1})$$

$$(\varepsilon - \varepsilon_p)a_{\alpha,0} = -i\xi_p^0 \sum_{\beta,\beta'} \epsilon_{\alpha\beta\beta'} \delta^\beta a_{\beta',0} + \sum_{\gamma,n} t_{\alpha,\gamma}(\theta_n)a_{\gamma,n}, \quad (\text{A2})$$

where $\alpha, \beta \in \{x, y, z\}$, while $\gamma \in \{s, x, y, z\}$, and we have employed the shorthand notation $t_{\alpha,\beta}(\theta_n) := t_{\alpha,\beta}^{0n}$, where the constant $t_{s,s} := t_{s,s}^{0n}$ in particular, and $t_{\alpha,\beta}(\theta_n) := t_{\alpha,\beta}^{nn'}$, to emphasize the local bending strength at each site. The p -orbital energy is denoted ε_p and the s -orbital energy ε_s . With the aim to obtain the secular equation for site 0, we first replace $0 \rightarrow n$ and $n \rightarrow n'$ in (A1) and (A2) and insert the result into the secular equations for $a_{\alpha,0}$, neglecting the s -orbital hopping [contained in the first term in the right-hand side of Eq. (A1)]. This leads to the wave function of the NNN model, mentioned in the main text with the following expression:

$$(\varepsilon - \varepsilon_p - \varepsilon'')a_{z,0} = A_n + A_{nn} + B_{nn} + C_{nn}. \quad (\text{A3})$$

The next section lists these components individually.

2. Full terms for the 4-orbital NNN hopping model

Here we state the effective terms for the 4-orbital model, where the hybridization energy of the σ orbitals is given by

$$\varepsilon_\sigma = -\frac{1}{\varepsilon_s} \sum_n [t_{x,s}(\theta_n)t_{s,x}(\theta_n) + t_{y,s}(\theta_n)t_{s,y}(\theta_n)]. \quad (\text{A4})$$

The nearest-neighbor hopping term is given by

$$A_n := \sum_n t_{z,z}(\theta_n)a_{z,n}. \quad (\text{A5})$$

The effective NNN terms without spin flip are

$$\begin{aligned} A_{nn} := & -\frac{1}{\varepsilon_s} \sum_{n,n' \neq 0} t_{z,s}(\theta_n)t_{s,z}(\theta_{n'})a_{z,n'} \\ & + \frac{1}{\varepsilon_\sigma} \sum_{n,n' \neq 0} [t_{z,x}(\theta_n)t_{x,z}(\theta_{n'}) + t_{z,y}(\theta_n)t_{y,z}(\theta_{n'})]a_{z,n'} \\ & - \left(\frac{\xi_p}{\varepsilon_s}\right)^2 \frac{1}{\varepsilon_s} \sum_{n,n' \neq 0} [t_{x,s}(\theta_n)t_{s,x}(\theta_{n'}) + t_{y,s}(\theta_n)t_{s,y}(\theta_{n'})] \\ & \times a_{z,n'}. \end{aligned}$$

The first and second terms describe a hopping from a p_z orbital to either an s , p_x , or p_y orbital, followed by

a hopping to an NNN p_z orbital. The last term describes an on-site SOC transition from the p_z orbitals to the p_x or p_y orbitals, followed by two hoppings and a transition back to a p_z orbital at a NNN site, again without affecting the spin as a result. Due to the quadratic order in ξ_p , this term is small. The two spin-dependent NNN terms are given by

$$B_{nn} := i \frac{\xi_p}{(\varepsilon_\sigma)^2} \sum_{n,n' \neq 0} \{ \hat{s}^y [t_{z,x}(\theta_n) t_{x,x}(\theta_{n'}) + t_{z,y}(\theta_n) t_{y,x}(\theta_{n'})] - \hat{s}^x [t_{z,x}(\theta_n) t_{x,y}(\theta_{n'}) + t_{z,y}(\theta_n) t_{y,y}(\theta_{n'})] \} a_{z,n'} \\ - i \frac{\xi_p}{(\varepsilon_\sigma)^2} \sum_{n,n' \neq 0} \{ \hat{s}^y [t_{x,x}(\theta_n) t_{x,z}(\theta_{n'}) + t_{x,y}(\theta_n) t_{y,z}(\theta_{n'})] - \hat{s}^x [t_{y,x}(\theta_n) t_{x,z}(\theta_{n'}) + t_{y,y}(\theta_n) t_{y,z}(\theta_{n'})] \} a_{z,n'} \\ - i \frac{\xi_p}{\varepsilon_\sigma \varepsilon_s} \sum_{n,n' \neq 0} \{ \hat{s}^y [t_{z,s}(\theta_n) t_{s,x}(\theta_{n'}) - t_{x,s}(\theta_n) t_{s,z}(\theta_{n'})] - \hat{s}^x [t_{z,s}(\theta_n) t_{s,y}(\theta_{n'}) - t_{y,s}(\theta_n) t_{s,z}(\theta_{n'})] \} a_{z,n'}, \quad (\text{A6})$$

$$C_{nn} = \frac{\xi_p^2}{(\varepsilon - \varepsilon_p)^2} \frac{1}{\varepsilon - \varepsilon_s} i \hat{s}_z \sum_{n,n' \neq 0} [t_{x,s}(\theta_n) t_{s,y}(\theta_{n'}) - t_{y,s}(\theta_n) t_{s,x}(\theta_{n'})] a_{z,n'} + \frac{\xi_p^2}{(\varepsilon - \varepsilon_p)^3} i \hat{s}_z \\ \times \sum_{n,n' \neq 0} [t_{x,x}(\theta_n) t_{x,y}(\theta_{n'}) - t_{y,x}(\theta_n) t_{x,x}(\theta_{n'}) - t_{y,y}(\theta_n) t_{y,x}(\theta_{n'}) + t_{x,y}(\theta_n) t_{y,y}(\theta_{n'})] a_{z,n'}, \quad (\text{A7})$$

where higher orders of ξ_p are omitted. As opposed to those matrix elements entering B_{nn} , the term C_{nn} stays nonzero even without bending. B_{nn} has a similar effective order as C_{nn} ; it describes hopping among next-nearest neighbors, followed by an on-site spin flip, resulting in linear order in ξ_p , but quadratic order in the hopping matrix elements. The same holds true for (A6), because the different matrix elements are unequal in the case of $\theta_n \neq \theta_{n'}$. For uniaxial deformations this is always the case, due to the different orientations of the bonds in the lattice and the resulting bending. The NNN hopping terms in (A6) from site 0 back to itself cause the aforementioned energy shift

of the p_z orbitals

$$\varepsilon'' \approx \frac{1}{\varepsilon_\sigma} \sum_n [t_{z,x}(\theta_n) t_{x,z}(\theta_n) + t_{z,y}(\theta_n) t_{y,z}(\theta_n)] + \frac{1}{\varepsilon_s} \sum_n t_{z,s}(\theta_n) t_{s,z}(\theta_n), \quad (\text{A8})$$

due to the hybridization of the in-plane and out-of-plane orbitals. If the edge sites of a graphene sample are not passivated with hydrogen atoms, the energy shift is approximately zero. However, the third term in (A8) largely overestimates the energy shift for passivated edge atoms by several orders of magnitude. The reason is that the sp^2 hybridization of the hydrogen atoms at the edge sites in the case of passivation shifts the energy of the hydrogen s orbitals, such that the contribution is reduced.

3. Full terms for the 9-orbital NNN hopping model

We extend the formalism of Sec. II C by adding the interaction of the d orbitals, which hybridize with the in-plane p orbitals in deformed graphene [41,42]. While the d orbitals are separated from the p orbitals by the energy $\varepsilon_d \approx 10$ eV, the energy separation of the s and d orbitals is ~ 20 eV, such that the s - d coupling can be safely neglected.

The secular equations for the 9-orbital model are given by (A1), together with

$$(\varepsilon - \varepsilon_p) a_{\alpha,0} = \sum_{\alpha'} \Lambda_{\alpha}^{\alpha'} a_{\alpha',0} + \sum_{\alpha',n} t_{\alpha,\alpha'}(\theta_n) a_{\alpha',n} + \sum_n t_{\alpha,s}(\theta_n) a_{s,n} + \sum_{\delta,n} t_{\alpha,\delta}(\theta_n) a_{\delta,n}, \quad (\text{A9})$$

$$(\varepsilon - \varepsilon_d) a_{\delta,0} = \sum_{\delta'} \Upsilon_{\delta}^{\delta'} a_{\delta',0} + \sum_{n,\alpha} t_{\delta,\alpha}(\theta_n) a_{\alpha,n} + \sum_{\delta',n} t_{\delta,\delta'}(\theta_n) a_{\beta',n}, \quad (\text{A10})$$

where the indices $\alpha, \alpha' \in \{x, y, z\}$ denote the p orbitals and $\delta, \delta' \in \{xz, yz, xy, z^2, x^2 - y^2\}$ the d orbitals. The matrix elements Λ_{ν}^{μ} and Υ_{ν}^{μ} denote the p -orbital atomistic SOC given in (1) and the d -orbital SOC in (2), respectively.

4. Full terms for the 9-band model

The equations (A1), (A9), and (A10) can be used analogously to (A1) and (A2) to find an effective NNN hopping from a p_z orbital at site 0 to a p_z orbital at its NNN sites n' , leading to

$$(\varepsilon - \varepsilon_p) a_{z,0} = \sum_{\alpha} \Lambda_{\alpha}^{\alpha} \frac{1}{\varepsilon_\sigma} \left(\sum_{\alpha'} \Lambda_{\alpha}^{\alpha'} a_{\alpha',0} + \sum_n \sum_{\alpha'} t_{\alpha,\alpha'}(\theta_n) a_{\alpha',n} + \sum_n \sum_{\beta} t_{\alpha,\beta}(\theta_n) a_{\beta,n} \right) \\ + \sum_{\alpha} \sum_n t_{z,\alpha}(\theta_n) \frac{1}{\varepsilon_\sigma} \left(\sum_{\alpha'} \Lambda_{\alpha}^{\alpha'} a_{\alpha',0} + \sum_{n'} \sum_{\alpha'} t_{\alpha,\alpha'}(\theta_{n'}) a_{\alpha',n'} + \sum_{n'} \sum_{\beta} t_{\alpha,\beta}(\theta_{n'}) a_{\beta,n'} \right) \\ + \sum_{\beta} \sum_n t_{z,\beta}(\theta_n) \frac{1}{\varepsilon - \varepsilon_d} \left(\sum_{\beta'} \Upsilon_{\beta}^{\beta'} a_{\beta',n} + \sum_{n'} \sum_{\alpha} t_{\beta,\alpha}(\theta_{n'}) a_{\alpha,n'} + \sum_{n'} \sum_{\beta'} t_{\beta,\beta'}(\theta_{n'}) a_{\beta',n'} \right). \quad (\text{A11})$$

TABLE III. The Slater-Koster matrix elements for the relative angle θ of the normals between orbital μ at site 1 and orbital ν at site 0 for the s and three p orbitals. The spatial orientation of the orbitals is mainly given by the angle ϕ . Due to the different parity of the s and p orbitals, some matrix elements are similar up to a sign.

μ_1/ν_0	s	p_x	p_y	p_z
s	$V_{ss\sigma}$	$V_{sp\sigma} \cos(\phi) \cos(\theta)$	$V_{sp\sigma} \cos(\theta) \sin(\phi)$	$V_{sp\sigma} \sin(\theta)$
p_x	$-V_{sp\sigma} \cos(\phi) \cos(\theta)$	$V_{pp\pi} \sin(\phi)^2 + [V_{pp\sigma} + (V_{pp\pi} - V_{pp\sigma}) \sin(\theta)^2] \times \cos(\phi)^2$	$(V_{pp\sigma} - V_{pp\pi}) \cos(\phi) \cos(\theta)^2 \sin(\phi)$	$(V_{pp\sigma} - V_{pp\pi}) \cos(\theta) \cos(\phi) \times \sin(\theta)$
p_y	$-V_{sp\sigma} \cos(\theta) \sin(\phi)$	$(V_{pp\sigma} - V_{pp\pi}) \cos(\phi) \cos(\theta)^2 \times \sin(\phi)$	$V_{pp\pi} \cos(\phi)^2 + (V_{pp\sigma} + (V_{pp\pi} - V_{pp\sigma}) \sin(\theta)^2) \times \sin(\phi)^2$	$(V_{pp\sigma} - V_{pp\pi}) \cos(\theta) \sin(\theta) \times \sin(\phi)$
p_z	$-V_{sp\sigma} \sin(\theta)$	$(V_{pp\sigma} - V_{pp\pi}) \cos(\theta) \cos(\phi) \times \sin(\theta)$	$(V_{pp\sigma} - V_{pp\pi}) \cos(\theta) \sin(\theta) \sin(\phi)$	$(V_{pp\sigma} - V_{pp\pi}) \sin(\theta)^2 + V_{pp\pi}$

The third term in the first line of (A11) leads to the Rashba-type SOC, because the bending of the ribbon lifts the symmetry along the surface normal of the graphene plane. It also describes terms of third order in either the atomistic SOC or the hopping. Those will not be considered in this perturbation theory. The eighth term, in the last line, leads to the effective NNN hopping. The term A_{nn} is given by

$$A_{nn}^D = -\frac{1}{\varepsilon_d} \sum_{n,n' \neq 0} [t_{z,xz}(\theta_n) t_{xz,z}(\theta_{n'}) + t_{z,yz}(\theta_n) t_{yz,z}(\theta_{n'})] a_{z,n'}. \quad (\text{A12})$$

Due to the coupling of the p_z and d orbitals, an additional energy shift is obtained from (A12):

$$\varepsilon_d'' = \frac{1}{\varepsilon_d} \sum_n [t_{z,xz}(\theta_n) t_{xz,z}(\theta_n) + t_{z,yz}(\theta_n) t_{yz,z}(\theta_n)] \approx \frac{3V_{pd\pi}^2}{\varepsilon_d}. \quad (\text{A13})$$

Due to the p -orbital atomistic SOC it follows for the effective Rashba-type SOC term $B_{nn}^{D,1}$ that

$$B_{nn}^{D,1} = \sum_\alpha \Lambda_z^\alpha \frac{1}{\varepsilon_\sigma} \sum_n \sum_\beta t_{\alpha,\beta}(\theta_n) \frac{1}{\varepsilon_d} \sum_{n' \neq 0} t_{\beta,z}(\theta_{n'}) a_{z,n'}. \quad (\text{A14})$$

Using (1), $\Lambda_z^x = -i\hat{s}^y \xi_p$, $\Lambda_z^y = i\hat{s}^x \xi_p$, and $\Lambda_z^z = 0$ are obtained. Thus, the effective Rashba-type contribution among p_z

orbitals becomes

$$B_{nn}^{p_z} = -\frac{i\xi_p}{\varepsilon_\sigma \varepsilon_d} \sum_{n,n' \neq 0} \left[\hat{s}^y \left(\sum_\beta t_{x,\beta}(\theta_n) t_{\beta,z}(\theta_{n'}) \right) - \hat{s}^x \left(\sum_\beta t_{y,\beta}(\theta_n) t_{\beta,z}(\theta_{n'}) \right) \right] a_{z,n'}. \quad (\text{A15})$$

The full bending-induced d -orbital Rashba-type SOC for the effective 9-orbital model in (12) is given by $B_{nn}^D = B_{nn}^{p_z} + B_{nn}^{D,2}$. The second term is contained in the seventh term of (A11) (in the last line), which can be rewritten as

$$C_{nn}^D + B_{nn}^{D,2} = \sum_\beta \sum_n t_{z,\beta}(\theta_n) \frac{1}{(\varepsilon - \varepsilon_d)^2} \sum_{\beta'} \Upsilon_\beta^{\beta'} \times \sum_{n' \neq 0} t_{\beta',z}(\theta_{n'}) a_{z,n'}, \quad (\text{A16})$$

and is given by

$$B_{nn}^{D,2} = -\frac{i\xi_d}{\varepsilon_d^2} \sum_{n,n' \neq 0} \sum_{l=1}^3 v(l) [\hat{s}^y (t_{z,p(l,1)}(\theta_n) t_{p(l,2),z}(\theta_{n'}) - t_{z,p(l,2)}(\theta_n) t_{p(l,1),z}(\theta_{n'})) - \hat{s}^x (t_{z,q(l,1)}(\theta_n) t_{q(l,2),z}(\theta_{n'}) - t_{z,q(l,2)}(\theta_n) t_{q(l,1),z}(\theta_{n'}))] a_{z,n'}, \quad (\text{A17})$$

$$C_{nn}^D = -\frac{i\xi_d \hat{s}^z}{\varepsilon_d^2} \sum_{n,n' \neq 0} \sum_{l=1}^2 w(l) [t_{z,r(l,1)}(\theta_n) t_{r(l,2),z}(\theta_{n'}) - t_{z,r(l,2)}(\theta_n) t_{r(l,1),z}(\theta_{n'})] a_{z,n'} \quad (\text{A18})$$

TABLE IV. The Slater-Koster matrix elements for the relative angle θ of the normals between orbital μ at site 1 and orbital ν at site 0 for the p_x and the five d orbitals.

μ_1/ν_0	p_x
d_{xz}	$\sin(\theta) [-\sqrt{3}V_{pd\sigma} \cos(\theta)^2 + V_{pd\pi} [\cos(\theta)^2 - \sin(\theta)^2]] \cos(\phi)^2 - V_{pd\pi} \sin(\phi)^2]$
d_{yz}	$(2V_{pd\pi} - \sqrt{3}V_{pd\sigma}) \sin(\theta) \cos(\theta)^2 \sin(\phi) \cos(\phi)$
d_{xy}	$\frac{1}{2} \cos(\theta) \{-2V_{pd\pi} [\cos(\phi)^2 - \sin(\phi)^2] \sin(\phi) + 2 \sin(\phi) \cos(\phi)^2 [\sqrt{3}V_{pd\sigma} \cos(\theta)^2 + 2V_{pd\pi} \sin(\theta)^2]\}$
d_{z^2}	$\frac{1}{4} \cos(\theta) \cos(\phi) \{V_{pd\sigma} - 3V_{pd\sigma} [\cos(\theta)^2 - \sin(\theta)^2] - 4\sqrt{3} \sin(\theta)^2\}$
$d_{x^2-y^2}$	$\frac{1}{2} \cos(\theta) \cos(\phi) \{2V_{pd\pi} + (\sqrt{3}V_{pd\sigma} - 2V_{pd\pi}) \cos(\theta)^2 [\cos(\theta)^2 - \sin(\theta)^2]\}$

TABLE V. The Slater-Koster matrix elements for the relative angle θ of the normals between orbital μ at site 1 and orbital ν at site 0 for the p_y and the five d orbitals.

μ_1/ν_0	p_y
d_{xz}	$(2V_{pd\pi} - \sqrt{3}V_{pd\sigma}) \cos(\theta)^2 \sin(\theta) \sin(\phi) \cos(\phi)$
d_{yz}	$\sin(\theta)[-V_{pd\pi} \cos(\phi)^2 + \{-\sqrt{3}V_{pd\sigma} \cos(\theta)^2 + V_{pd\pi}[\cos(\theta)^2 - \sin(\theta)^2]\} \sin(\phi)^2]$
d_{xy}	$\frac{1}{2} \cos(\theta)\{V_{pd\pi} \cos(\phi) + V_{pd\pi} \cos(3\phi) + [\sqrt{3}V_{pd\sigma} \cos(\theta)^2 + 2V_{pd\pi} \sin(\theta)^2]2 \sin(\phi)^2 \cos(\phi)\}$
d_{z^2}	$\frac{1}{4} \cos(\theta)\{V_{pd\sigma} - 3V_{pd\sigma}[\cos(\theta)^2 - \sin(\theta)^2] - 4\sqrt{3}V_{pd\pi} \sin(\theta)^2\} \sin(\phi)$
$d_{x^2-y^2}$	$\frac{1}{2} \cos(\theta)\{-4V_{pd\pi} \cos(\phi)^2 + [\cos(\phi)^2 - \sin(\phi)^2][\sqrt{3}V_{pd\sigma} \cos(\theta)^2 + 2V_{pd\pi} \sin(\theta)^2]\} \sin(\phi)$

for p_z orbitals. For this compact notation,

$$\begin{aligned}
[p(l, 1), p(l, 2)] &\in \{(yz, xy), (xz, x^2 - y^2), (xz, z^2)\}, \\
[q(l, 1), q(l, 2)] &\in \{(xy, xz), (yz, x^2 - y^2), (yz, z^2)\}, \\
[r(l, 1), r(l, 2)] &\in \{(xz, yz), (xy, x^2 - y^2)\} \quad (A19)
\end{aligned}$$

are introduced, which denote all of the pairs of orbitals relevant in the respective terms. The factors $v(l) \in \{1, 1, \sqrt{3}\}$ and $w(l) \in \{1, 2\}$ arise due to the numerical factors in the atomistic SOC operator (2). The bending-induced d -orbital SOC in (A17) is small, due to the second-order hopping in the energetically separate d orbitals and because the bending-induced hopping matrix elements are small for small θ . It is important, however, that $B_{nn}^{D,2} \sim \xi_d$. The effective form of the intrinsic SOC in (A18) contains a dominant contribution, given by (14). Although C_{nn}^D has the same appearance as $B_{nn}^{D,2}$, the contribution to the spin alignment of the former is much more relevant, because the matrix elements $t_{xz,z}(\theta)$ and $t_{yz,z}(\theta)$ are much larger than $t_{xy,z}(\theta)$ or $t_{x^2-y^2,z}(\theta)$.

APPENDIX B: SEMIANALYTIC DERIVATION OF THE SPIN-TILT DEPENDENCE ON THE SOC PARAMETER

In this section, the functions describing the dependency of the spin tilting on the SOC strength are computed more thoroughly. First, the hopping matrix elements $t_{i,j}(\theta)$ in the terms $B_{nn}^{(D)}$, etc., are expanded up to second order in θ . Then, the relative angle ϕ of the local surface normal $\vec{v}$ and the vector $\langle \hat{s} \rangle$ containing, e.g., the spin expectation value in the y direction $B_{nn}^{(D)}$ and in the z direction, $C_{nn}^{(D)}$, is evaluated as in (8).

For a full spin tilt, the condition $\arccos 0 = \frac{\pi}{2}$ is used to solve (8) for $\theta \sim 1/R^c$. For the 4-orbital model, it is $\langle \hat{s} \rangle = (0, B_{nn}, C_{nn})$, leading to

$$1/R^c \sim \frac{a + b\xi}{c + d\xi + \sqrt{e + f\xi}}. \quad (B1)$$

TABLE VI. The Slater-Koster matrix elements for the relative angle θ of the normals between orbital μ at site 1 and orbital ν at site 0 for the p_z and the five d orbitals.

μ_1/ν_0	p_z
d_{xz}	$\{\sqrt{3}V_{pd\sigma} \sin(\theta)^2 + V_{pd\pi}[\cos(\theta)^2 - \sin(\theta)^2]\} \cos(\phi) \cos(\theta)$
d_{yz}	$\{\sqrt{3}V_{pd\sigma} \sin(\theta)^2 + V_{pd\pi}[\cos(\theta)^2 - \sin(\theta)^2]\} \sin(\phi) \cos(\theta)$
d_{xy}	$(2V_{pd\pi} - \sqrt{3}V_{pd\sigma}) \cos(\phi) \sin(\theta) \cos(\theta)^2 \sin(\phi)$
d_{z^2}	$-\frac{1}{4} \sin(\theta)(V_{pd\sigma} + 4\sqrt{3}V_{pd\pi} \cos(\theta)^2 - 3V_{pd\sigma}[\cos(\theta)^2 - \sin(\theta)^2])$
$d_{x^2-y^2}$	$\frac{1}{2}(2V_{pd\pi} - \sqrt{3}V_{pd\sigma})[\cos(\phi)^2 - \sin(\phi)^2] \cos(\theta)^2 \sin(\theta)$

For the 9-orbital model, it is $\langle \hat{s} \rangle = (0, B_{nn} + B_{nn}^D, C_{nn} + C_{nn}^D)$. Under the condition $\xi_d/\xi_d^0 = 1$, this leads to

$$1/R^c \sim \frac{\sum_{i=0}^2 a_i \xi^i}{\sum_{i=0}^2 b_i \xi^i + \sqrt{\sum_{i=0}^4 c_i \xi^i}}, \quad (B2)$$

where $\xi = \xi_p/\xi_p^0$ and under the condition $\xi_p/\xi_p^0 = 1$, this leads to

$$1/R^c \sim \frac{a_0 + a_1 \xi}{b_0 + b_1 \xi + \sqrt{c_0 + c_1 \xi + c_2 \xi^2}}, \quad (B3)$$

where $\xi = \xi_d/\xi_d^0$. As indicated in Fig. 5(b), these functions are then fitted to the tilting of the spin. Only keeping the dominant terms, the spin tilting of the 4- and 9-orbital models is described by the functions

$$F_4^{\xi_p}(\xi) = a\sqrt{\xi}, \quad (B4)$$

$$F_9^{\xi_p}(\xi) = \frac{a + b\xi^2}{c + d\xi + \sqrt{e\xi + f\xi^3}}, \quad (B5)$$

$$F_9^{\xi_d}(\xi) = \frac{a + b\xi}{c + d\xi + \sqrt{e + f\xi}}, \quad (B6)$$

where ξ is the dimensionless SOC parameter indicated by the superscript.

APPENDIX C: SLATER-KOSTER MATRIX ELEMENTS FOR RELATIVE ANGLES

Various different approaches for computing the two-center approximation integrals can be found in the literature [51–54]. For specific purposes, some are more suitable than others. An approach by Elena and Meister [51] was used in this work, which allows one to obtain the transition matrix elements when rotated with respect to each other, which is particularly useful in bending computations. The results are listed in Tables III, IV, V, and VI.

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