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Multiband treatment of quantum transport in anisotropic semiconductors: Non-equilibrium Green's function

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A R T I C L E   I N F O

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A B S T R A C T

Using the non-equilibrium Green's function and anti-bonding orbital model, a multiband treatment of quantum transport in an anisotropic semiconductor (Si-based) system is developed. In this study, we adopt Chiang's boundary treatment of the open boundary system into the non-equilibrium Green's function framework, and then an easy and powerful multiband treatment method is developed to solve the transmission coefficient of Si-based semiconductor quantum structures.

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1. Introduction

Tunneling in semiconductor quantum structures has been attracting considerable interest and has been investigated intensively over the last two decades [1–3]. However, it has been widely recognized that the single-band model is insufficient to simulate quantum transport in material systems that are currently under investigation [4,5]. For example, several investigations have demonstrated that the X (or L)-valley energy plays a significant role in the transport, specifically for the indirect-gap (anisotropic) semiconductor structures [6–9]. That is one of the reasons that have prompted a number of researchers to include realistic band structures in quantum transport simulations. For this purpose, a multiband calculation technique, namely an anti-bonding orbital (ABO) model, had been proposed to calculate realistic conduction band structures [9,10]. In this study, we will propose a sophisticated quantum transport model based on a non-equilibrium Green's function (NEGF) [11–14] method taking a realistic ABO multiband structure into account.

In the past a large number of studies had appeared where different kinds of Green's functions were calculated by the iterative methods available [15–17]. Iterative procedures are suitable to accomplish this task, but most of them have in common a relatively slow convergence [18,19]. Furthermore, the other calculating method for Green's functions is based on the Dyson equation treatment of the open system boundaries developed by Caroli et al. and subsequently used by a number of authors [20–22]. This approach calculates the boundary self-energies in the device by including the coupling of the contacts (or reservoirs) to the device exactly using Dyson's equation. However, in Dyson's approach the matrix algebra is very tricky in the multiband treatment for Green's functions. The major drawback of this method is that the boundary conditions become extremely complicated to solve when many bands are involved.

In the previous paragraph, the drawback of the iterative method and Dyson's approach could be shown by the boundary treatment of another method (Chiang et al. 1993) [9]. The method proposed by Chiang et al. is based on the ABO framework and directly solved in the ABO Hamiltonian of the entire structure to obtain the transmission coefficient. In this study,

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we will adopt Chiang's boundary treatment of the open boundary system into the NEGF framework, and then an easy and powerful multiband NEGF method will be developed to solve the transmission coefficient of Si-based semiconductor quantum structures.

2. Theoretical method

We confine ourselves to the analysis of electron transport in the [001], [111], and [110] directions in two-dimensional Si-based microstructures. Then we can use an ABO model with a basis of four ABOs per lattice site (s, p_x, p_y, p_z) assuming a second nearest-neighbor approximation [9,10].

2.1. Anti-bonding orbital model

Basically, the ABO model is a tight-binding-like scheme with α-like ($\alpha = s, p_x, p_y, p_z$) unit-cell-scale ABO basis functions. In an analytical formalism, the ABO matrix elements can be written as [10]

$$\mathbf{H}_{\text{ABO}}(\mathbf{k})_{\alpha',\alpha} = \langle \mathbf{k}, \alpha' | \hat{\mathbf{H}} | \mathbf{k}, \alpha \rangle = \sum_{j=0}^{18} e^{i\mathbf{k}\cdot\mathbf{R}_j} \in_{\alpha',\alpha}(j), \tag{1}$$

where $\mathbf{k}$ is a wave vector, $\mathbf{R}_j$ with $j = 0$–18 is the position vector of the on-site lattice ($j = 0$), one of the 12 first nearest-neighbor lattices ($j = 1$–12), or one of the 6 nearest-neighbor lattices ($j = 13$–18), $\in_{\alpha',\alpha}(j)$ is an interaction parameter between ABOs of symmetry types α' (located at the relative origin, $\mathbf{R}'$) and α (located at one of the lattice sites $\mathbf{R} = \mathbf{R}_j + \mathbf{R}'$ with $j = 1$–18), and $|\mathbf{k}, \alpha\rangle$ denotes the Bloch wavefunction. The Bloch wavefunction can be written as

$$|\mathbf{k}, \alpha\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R}, \alpha\rangle, \tag{2}$$

where $|\mathbf{R}, \alpha\rangle$ denotes the α-like ABO at lattice site $\mathbf{R}$ and N is the number of unit cells. As shown in the Appendix, a total of eleven interaction parameters ($\in_{\alpha',\alpha}$) exist, namely, E_s, E_p, E_{ss}, E_{sx}, E_{xx}, E_{xy}, E_{zz}, V_{ss}, V_{sx}, V_{xx}, and V_{zz}. The first two parameters relate to the on-site anti-orbital energies, while the remaining parameters represent the nearest-neighbor interactions.

The ABO method is a tight-binding form with ABO basis. In the ABO framework, we describe the NEGF method briefly as follows.

2.2. Non-equilibrium Green's function method

We divide the heterostructure into three sections: a semi-infinite flat-band region on the left (L) with the wavefunction $|\psi; L\rangle$, a semi-infinite flat-band region on the right (R) with the wavefunction $|\psi; R\rangle$, and a central N-monolayer segment containing the heterointerfaces with the wavefunction $|\psi; 1\text{–}N\rangle$. The left and right sections are chosen to be regions with constant doping levels that are sufficiently far away from the heterostructures so that the potentials and compositions are constant; the wavefunction in these regions can therefore be described in terms of bulk-like plane-wave states.

We consider the heterostructure as a sequence of monolayer parallel to the heterostructures. The basis orbitals at lattice site $\mathbf{R} = (\mathbf{R}_\parallel, \sigma)$ may be written in the form $|\mathbf{R}_\parallel, \sigma, \alpha\rangle$, where σ is an integer monolayer label ($\sigma = 1, 2, \ldots, N$ in the central region), $\mathbf{R}_\parallel$ specifies the in-plane component of unit cell coordinates, and α ($=s, p_x, p_y, p_z$) labels the ABOs within a unit cell. Since the in-plane crystal momentum ($\mathbf{k}_\parallel$) is a good quantum number, the wavefunction of the whole structure may be written as [4]

$$|\psi\rangle = \sum_{\sigma,\alpha} F_{\sigma\alpha} |\mathbf{k}_\parallel, \sigma, \alpha\rangle, \tag{3}$$

where $|\mathbf{k}_\parallel, \sigma, \alpha\rangle$ is a planar orbital formed by taking Bloch sums of ABOs over the $N_\parallel$ unit cells in the σth monolayer:

$$|\mathbf{k}_\parallel, \sigma, \alpha\rangle = \frac{1}{\sqrt{N_\parallel}} \sum_{\mathbf{R}_\parallel} e^{i\mathbf{k}_\parallel\cdot\mathbf{R}_\parallel} |\mathbf{R}_\parallel, \sigma, \alpha\rangle.$$

Writing the Schrödinger equation $(H - E)|\psi\rangle = 0$ in the planar orbital basis, we obtain

$$H_{\sigma,\sigma-2}F_{\sigma-2} + H_{\sigma,\sigma-1}F_{\sigma-1} + \bar{H}_{\sigma,\sigma}F_\sigma + H_{\sigma,\sigma+1}F_{\sigma+1} + H_{\sigma,\sigma+2}F_{\sigma+2} = 0, \tag{4}$$

where F_σ denotes a four-dimensional column vector whose components are $F_{\sigma\alpha}$, i.e.,

$$F_\sigma = \begin{bmatrix} F_{\sigma 1} \\ F_{\sigma 2} \\ F_{\sigma 3} \\ F_{\sigma 4} \end{bmatrix},$$

and $H_{\sigma,\sigma'}$ and $\bar{H}_{\sigma,\sigma}$ are 4×4 matrices whose elements are given by, respectively,

$$(\bar{H}_{\sigma,\sigma})_{\alpha,\alpha'} = \langle \mathbf{k}_\parallel, \sigma, \alpha | (H - E) | \mathbf{k}_\parallel, \sigma, \alpha' \rangle$$

and

$$(H_{\sigma,\sigma'})_{\alpha,\alpha'} = \langle \mathbf{k}_{\parallel}, \sigma, \alpha | H | \mathbf{k}_{\parallel}, \sigma', \alpha' \rangle.$$

Note that the interaction between two planar orbitals does not extend beyond the second nearest layer, i.e.,

$$H_{\sigma,\sigma'} = 0 \quad \text{for } |\sigma - \sigma'| > 2.$$

The Schrödinger equation can also be written in the transfer-matrix form [4,9]:

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -H^{-1}_{\sigma,\sigma+2}H_{\sigma,\sigma-2} & -H^{-1}_{\sigma,\sigma+2}H_{\sigma,\sigma-1}H & -H^{-1}_{\sigma,\sigma+2}\bar{H}_{\sigma,\sigma} & -H^{-1}_{\sigma,\sigma+2}H_{\sigma,\sigma+1} \end{bmatrix} \begin{bmatrix} F_{\sigma-2} \\ F_{\sigma-1} \\ F_{\sigma} \\ F_{\sigma+1} \end{bmatrix} = \begin{bmatrix} F_{\sigma-1} \\ F_{\sigma} \\ F_{\sigma+1} \\ F_{\sigma+2} \end{bmatrix}. \tag{5}$$

The boundary conditions are such that we have a known incoming plane-wave state from the left region, no incoming states from the right, and unknown outgoing transmitted and reflected plane-wave states in the right and left regions, respectively. First, the available plane-wave states in the left and right regions can be found by noting that for a Bloch state

$$|k_{\perp}\rangle = \sum_{\sigma,\alpha} B_{\sigma\alpha}(k_{\perp}) |\mathbf{k}_{\parallel}, \sigma, \alpha\rangle, \tag{6}$$

where $B_{\sigma\alpha}$ is the tight-binding coefficient $F_{\sigma\alpha}$ at the semi-infinite flat-band region on the right and left bulk sides.

The tight-binding coefficients at the semi-infinite bulk sides must obey the relation

$$B_{\sigma} = e^{ik_{\perp}d} B_{\sigma-1}, \tag{7}$$

where d is the distance between monolayers and $k_{\perp}$ is the component of the crystal momentum along the growth direction. Note that B_{σ} denotes a four-dimensional column vector whose components are $B_{\sigma\alpha}$. Thus,

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -H^{-1}_{\sigma,\sigma+2}H_{\sigma,\sigma-2} & -H^{-1}_{\sigma,\sigma+2}H_{\sigma,\sigma-1} & -H^{-1}_{\sigma,\sigma+2}\bar{H}_{\sigma,\sigma} & -H^{-1}_{\sigma,\sigma+2}H_{\sigma,\sigma+1} \end{bmatrix} \begin{bmatrix} B_{\sigma-2} \\ B_{\sigma-1} \\ B_{\sigma} \\ B_{\sigma+1} \end{bmatrix} = e^{-ik_{\perp}d} \begin{bmatrix} B_{\sigma-2} \\ B_{\sigma-1} \\ B_{\sigma} \\ B_{\sigma+1} \end{bmatrix}. \tag{8}$$

By solving the eigenvalue problem for the transfer matrix in Eq. (8), we can obtain a set of 16 complex eigenvalues $\{k_{\perp,j}; j = 1, 2, \ldots, 16\}$ and their associated eigenvectors $[B_{\sigma-2,j}, B_{\sigma-1,j}, B_{\sigma,j}, B_{\sigma+1,j}]^T$, where the superscript T denotes the matrix transpose.

We define that: $|k^{\beta}_{\perp}\rangle = \sum_{\sigma,\alpha} B^{\beta}_{\sigma\alpha} |\mathbf{k}_{\parallel}, \sigma, \alpha\rangle$ at bulk sites ($\beta = r, t$ for reflected and transmitted waves in the left and right regions, respectively),

$$[D^{\beta}_{\sigma,1}\ D^{\beta}_{\sigma,2}] = [B^{\beta}_{\sigma,1}B^{\beta}_{\sigma,2}B^{\beta}_{\sigma,3}B^{\beta}_{\sigma,4}B^{\beta}_{\sigma,5}B^{\beta}_{\sigma,6}B^{\beta}_{\sigma,7}B^{\beta}_{\sigma,8}] \quad \text{for } \beta = r, \text{ and}$$
$$[D^{\beta}_{\sigma,1}\ D^{\beta}_{\sigma,2}] = [B^{\beta}_{\sigma,9}B^{\beta}_{\sigma,10}B^{\beta}_{\sigma,11}B^{\beta}_{\sigma,12}B^{\beta}_{\sigma,13}B^{\beta}_{\sigma,14}B^{\beta}_{\sigma,15}B^{\beta}_{\sigma,16}] \quad \text{for } \beta = t.$$

The Green's function of the device is simply defined as [11–14]

$$G_d = \left(E - H_d - \sum_{L} - \sum_{R} \right)^{-1}, \tag{9}$$

where H_d is the Hamiltonian for the device (d) region and $\Sigma_{L,R}$ are the self-energies for the left (L) and right (R) contacts (or reservoirs), which can be expressed as [9]

$$H_d = \begin{bmatrix} H_{-1,-1} & H_{-1,0} & H_{-1,1} & 0 & \cdots & \cdots & \cdots & 0 \\ H_{0,-1} & H_{0,0} & H_{0,1} & H_{0,2} & 0 & \cdots & \cdots & 0 \\ H_{1,-1} & H_{1,0} & H_{1,1} & H_{1,2} & H_{1,3} & 0 & \cdots & 0 \\ 0 & H_{2,0} & H_{2,1} & H_{2,2} & H_{2,3} & H_{2,4} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & H_{N,N-2} & H_{N,N-1} & H_{N,N} & H_{N,N+1} & H_{N,N+2} \\ 0 & \cdots & \cdots & 0 & H_{N+1,N-1} & H_{N+1,N} & H_{N+1,N+1} & H_{N+1,N+2} \\ 0 & \cdots & \cdots & \cdots & 0 & H_{N+2,N} & H_{N+2,N+1} & H_{N+2,N+2} \end{bmatrix},$$

$$\Sigma_L = \begin{bmatrix} H_{-1,-3} & H_{-1,-2} \\ 0 & H_{0,-2} \end{bmatrix} \begin{bmatrix} D^r_{-3,1} & D^r_{-3,2} \\ D^r_{-2,1} & D^r_{-2,2} \end{bmatrix} \begin{bmatrix} D^r_{-1,1} & D^r_{-1,2} \\ D^r_{0,1} & D^r_{0,2} \end{bmatrix}^{-1},$$

$$\Sigma_R = \begin{bmatrix} H_{N+1,N+3} & 0 \\ H_{N+2,N+3} & H_{N+2,N+4} \end{bmatrix} \begin{bmatrix} D^t_{N+3,1} & D^t_{N+3,2} \\ D^t_{N+4,1} & D^t_{N+4,2} \end{bmatrix} \begin{bmatrix} D^t_{N+1,1} & D^t_{N+1,2} \\ D^t_{N+2,1} & D^t_{N+2,2} \end{bmatrix}^{-1}.$$

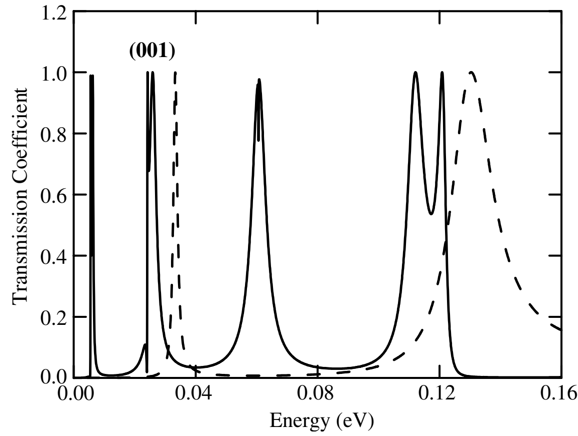

Fig. 1. Transmission coefficients for a Ge–Si–Ge (001) double-barrier structure with $N_{BR} = 2$ and $N_W = 24$ monolayers (sandwiched between n^--Si regions) for two independently incident electrons with $\mathbf{k}_\parallel = (0, 0)$ (solid curve) and $\mathbf{k}_\parallel = (k_0, 0)$ (dashed curve).

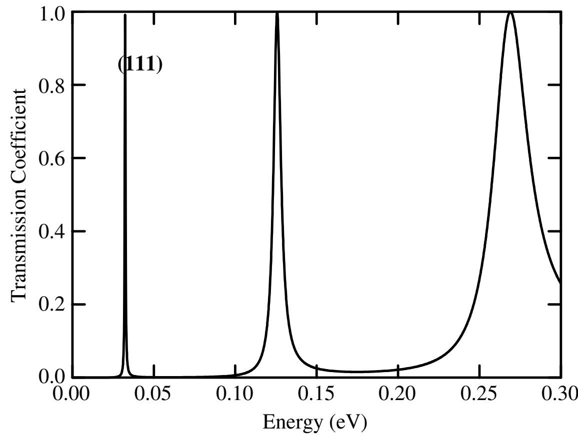

Fig. 2. Transmission coefficients for a $Si_{0.15}Ge_{0.85}$–Si–$Si_{0.15}Ge_{0.85}$ (111) double-barrier structure with $N_{BR} = 2$ and $N_W = 18$ monolayers (sandwiched between n^--Si regions) for incident electron with $\mathbf{k}_\parallel = (0, (2/\sqrt{6})k_0)$.

Within the NEGF formalism, the transmission coefficient $T(E)$ is written as [11–14]

$$T(E) = \text{Trace}[\Gamma_L G_d \Gamma_R G_d^+], \tag{10}$$

where the broadening factors are $\Gamma_{L,R} = i(\Sigma_{L,R} - \Sigma_{L,R}^+)$.

3. Results and discussion

Here we present calculated results for the $Si_{1-x}Ge_x$–Si–$Si_{1-x}Ge_x$ double-barrier structure (DBS) grown in three different orientations, (001), (111), and (110). The entire DBS is sandwiched between two n^--Si bulk regions. Through this study the doping concentration in the Si electrodes is assumed to be 10^{18} cm^{-3}. To understand the electron resonant-tunneling properties involving a multivalley semiconductor like Si, it is necessary to have a clear picture of the six equivalent ellipse pockets projected onto planes normal to various growth axes. The center positions of these ellipse pockets are located at $\mathbf{k}_\parallel = (0, 0), (0, \pm k_0)$, and $(\pm k_0, 0)$ for (001), $\mathbf{k}_\parallel = (\pm(2/\sqrt{6})k_0, 0)$, $(\pm(1/\sqrt{6})k_0, \pm(1/\sqrt{2})k_0)$, and $(\pm(1/\sqrt{6})k_0, \mp(1/\sqrt{2})k_0)$ for (111), and $\mathbf{k}_\parallel = (0, 0)$, $(\pm(1/\sqrt{2})k_0, 0)$, and $(0, \mp k_0')$ for (110), where $k_0 = 0.86\ (2\pi/a)$ and $k_0' = 0.142(\pi/a)$.

The (001) DBS consists of a Si quantum well of 24 monolayers sandwiched between two Ge barriers, each consisting of two monolayers. For $\mathbf{k}_\parallel = (k_0, 0)$ and $\mathbf{k}_\parallel = (0, 0)$, the corresponding barrier heights are 0.125 and 0.73 eV, respectively [9, 23]. Fig. 1 shows calculated transmission coefficients $T(E, \mathbf{k}_\parallel)$ of the (001) DBS for $\mathbf{k}_\parallel = (0, 0)$ (solid) and $\mathbf{k}_\parallel = (k_0, 0)$ (dashed).

The (111) DBS considered here consists of a Si quantum well of 18 monolayers sandwiched between two $Si_{0.15}Ge_{0.85}$ barriers, each consisting of two monolayers. Fig. 2 shows calculated transmission coefficients $T(E, \mathbf{k}_\parallel)$ of the (111) DBS for $\mathbf{k}_\parallel = (0, (2/\sqrt{6})k_0)$. The results for electrons derived from the other five valleys are equivalent due to symmetry. The barrier height for this case is 0.144 eV [9].

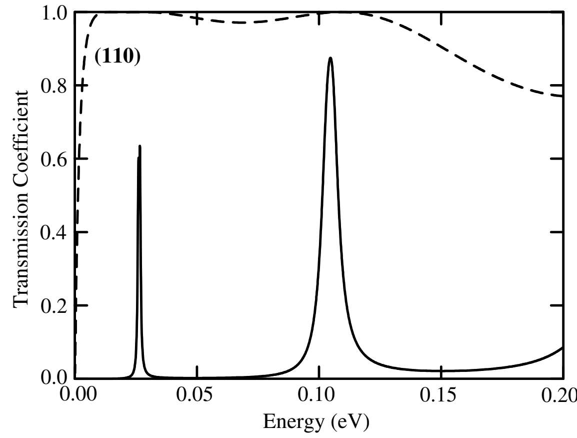

Fig. 3. Transmission coefficients for a $Si_{0.15}Ge_{0.85}$–Si–$Si_{0.15}Ge_{0.85}$ (110) double-barrier structure with $N_{BR} = 2$ and $N_W = 30$ monolayers (sandwiched between n^--Si regions) for two independently incident electrons with $\mathbf{k}_\parallel = (k'_0, 0)$ (solid curve) and $\mathbf{k}_\parallel = (0, (1/\sqrt{2})k_0)$ (dashed curve).

The (110) DBS considered here consists of a Si quantum well of 30 monolayers sandwiched between two $Si_{0.15}Ge_{0.85}$ barriers, each consisting of two monolayers. The minimum conduction-band energy in the barrier region is −0.12 eV for $\mathbf{k}_\parallel = (0, (1/\sqrt{2})k_0)$ and 0.28 eV for $\mathbf{k}_\parallel = (k'_0, 0)$ (with respect to the Si conduction-band minimum) [9]. Fig. 3 shows calculated transmission coefficients $T(E, \mathbf{k}_\parallel)$ of the (110) DBS for $\mathbf{k}_\parallel = (k'_0, 0)$ (solid) and $\mathbf{k}_\parallel = (0, (1/\sqrt{2})k_0)$ (dashed). Due to the absence of a resonant-tunneling barrier, we found no resonant-tunneling behavior for incident electron with $\mathbf{k}_\parallel = (0, (1/\sqrt{2})k_0)$.

Figs. 1–3 show almost the same figure shapes as those of Chiang et al. [9]. The drawback of Chiang's method is that the disposal of the plane-wave states in the right and left reservoirs becomes extremely complicated when many bands are involved [9]. Furthermore, Chiang's method required more computational effort. However, Chiang's method takes the full band structure into account, and its boundary treatment is straightforward. In this study, we conserve Chiang's advantage (boundary treatment), which is used inside the NEGF framework. Then an easy and powerful multiband NEGF method is developed to solve the transmission coefficient of Si-based semiconductor quantum structures. The proposed method is easy, but it can become quite sophisticated in quantum transport calculations and saves much computational effort. Moreover, the ABO model is a tight-binding-like framework, and thus the proposed framework in this study can be used in a tight-binding method with an atomic-orbital basis for quantum transport calculation.

4. Conclusions

We have developed the multiband treatment of quantum transport in an anisotropic semiconductor (Si-based) system using the non-equilibrium Green's function and anti-bonding orbital model. In this study, we have adopted Chiang's boundary treatment of the open boundary system into the non-equilibrium Green's function framework. Then an easy and powerful multiband treatment method has been developed to solve the transmission coefficient of Si-based semiconductor quantum structures. Importantly, the Green's function drawback of the iterative method and Dyson's approach could be shown by Chiang's boundary treatment.

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Appendix

The tight-binding Hamiltonian within the ABO basis for a bulk Si semiconductor (in the basis ordering: s, p_x, p_y, p_z) can be written as [10]

$$\mathbf{H}_{\mathrm{ABO}}(\mathbf{k}) = \begin{bmatrix} E_s + E_{ss}T_s + V_{ss}C_s & E_{sx}T_x + V_{sx}S_x & E_{sx}T_y + V_{sx}S_y & E_{sx}T_z + V_{sx}S_z \\ -E_{sx}T_x - V_{sx}S_x & E_p + E_x^{(1)} + E_x^{(2)} & E_{xy}T_{xy} & E_{xy}T_{xz} \\ -E_{sx}T_y - V_{sx}S_y & E_{xy}T_{xy} & E_p + E_y^{(1)} + E_y^{(2)} & E_{xy}T_{yz} \\ -E_{sx}T_z - V_{sx}S_z & E_{xy}T_{xz} & E_{xy}T_{yz} & E_p + E_z^{(1)} + E_z^{(2)} \end{bmatrix}, \quad \text{(A.1)}$$

where E_s and E_p are the on-site energies for the s- and p-like ABOs, respectively, $E_{\alpha,\beta}$ $(\alpha, \beta = s, x, y, z)$ denotes the first nearest-neighbor interaction energies, and $V_{\alpha,\beta}$ denotes the second nearest-neighbor interaction energies,

$$T_x = 4i\sin(k_xa/2)[\cos(k_ya/2) + \cos(k_za/2)],$$
$$T_y = 4i\sin(k_ya/2)[\cos(k_xa/2) + \cos(k_za/2)],$$
$$T_z = 4i\sin(k_za/2)[\cos(k_xa/2) + \cos(k_ya/2)],$$
$$T_{xx} = 4\cos(k_xa/2)[\cos(k_ya/2) + \cos(k_za/2)],$$
$$T_{yy} = 4\cos(k_ya/2)[\cos(k_xa/2) + \cos(k_za/2)],$$
$$T_{zz} = 4\cos(k_za/2)[\cos(k_xa/2) + \cos(k_ya/2)],$$
$$T_{xy} = -4\sin(k_xa/2)\sin(k_ya/2),$$
$$T_{xz} = -4\sin(k_xa/2)\sin(k_za/2),$$
$$T_{yz} = -4\sin(k_ya/2)\sin(k_za/2),$$
$$T_s = T_{xx} + T_{yy} + T_{zz},$$
$$S_x = 2i\sin(k_xa),$$
$$S_y = 2i\sin(k_ya),$$
$$S_z = 2i\sin(k_za),$$
$$C_x = 2\cos(k_xa),$$
$$C_y = 2\cos(k_ya),$$
$$C_z = 2\cos(k_za),$$
$$C_s = C_x + C_y + C_z.$$

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