

Electron Dynamics in Semiconducting Nanowires: A Real-Space, Polynomial-Expansion Approach

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We present a real-space, polynomial-expansion approach to electron dynamics in nanostructured semiconductors. The Chebyshev expansion method is employed for efficient calculation of time-evolution of single-electron wave function. Details of the formulation are described. The method is applied to the electron transport in nanostructured semiconductors such as Si nanowires. The mean-square displacement and diffusivity of electron in Si chains are obtained as functions of length of the chains. The results show clearly ballistic behavior of electron in the pure Si chain.

1. INTRODUCTION

Recent progress in nanotechnology has made electron dynamics in nanostructures extremely important. In order to design nanostructured circuit, nanowire is necessary. For example, FET that consists of one semiconducting single-wall carbon nanotube has been fabricated [1]. Recently, 1.3 nm diameter of Si nanowire has been made [2]. Electron transport in such nanoscale devices has shown essential differences in its mechanisms from those described by conventional approaches for bulk semiconductors. Most of the theoretical approaches to electron dynamics in bulk semiconductors have been based on the effective mass approximation, which has been quite successful for reproducing macroscopic properties of various semiconductors. However, the standard effective mass method cannot be applied to nanostructures, because the method describes only the envelope of electron wave functions and neglects interband electron tran-

sitions. Therefore, microscopic theories, such as the Kubo-Greenwood theorem [3] and Landauer formula, have been applied to the electron transport. In the mesoscopic or nanoscale systems, Landauer formula is often used for calculating electrical conductance of various systems in nanoscales [5, 6]. In the approach, the electron transmission probability needs to be calculated by, for example, the transfer matrix method or the non-equilibrium Green's function [4].

Alternative way to describe electron dynamics is the time dependent Schrödinger equation. In order to solve the time dependent Schrödinger equation, various methods have been proposed [7–9]. In the present study, we use the Heisenberg operator for electronic positions to calculate electron dynamics, following the idea that D. Mayou, S. Roche *et al.* have developed [10–16]. In Ref. [10], the authors calculated DC conductivity of a quasi-periodic system using the Kubo-Greenwood formula. They adopted the Chebyshev expansion for calculating efficiently the Heisenberg operator. The same technique has been applied to an analysis on the electron diffusivity in a grain boundary of SiC [17]. Here, we use similar technique for calculating electron diffusivity in silicon chain, as a model system of nanostructured semiconductor.

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2. THEORY

The time dependent Schrödinger equation is defined as

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle. \quad (1)$$

From Eq.(1), time evolution of an electronic state can be described as

$$|\Psi(t)\rangle = \exp\left(-i\hat{H}t/\hbar\right) |\Psi(t=0)\rangle, \quad (2)$$

where $|\Psi(t=0)\rangle$ is the initial state. In this study, we employ the tight-binding method and take atomic-like orbitals as initial states. Therefore Eq.(2) can be rewritten as

$$|\Psi_{i\alpha}(t)\rangle = \exp\left(-i\hat{H}t/\hbar\right) |i\alpha\rangle. \quad (3)$$

These i and α denote indices of an atom and its associated orbital, respectively. Here, $\exp\left(-i\hat{H}t/\hbar\right)$ is referred to as time evolution operator. As shown above, if this operator acts on the initial state, the state in a given time can be obtained.

The time-dependent electron diffusivity is defined as

$$D_i(t) = \frac{1}{t} \frac{\sum_{\alpha} \langle \Psi_{i\alpha}(t) | \hat{X}^2 | \Psi_{i\alpha}(t) \rangle}{\sum_{\alpha} \langle \Psi_{i\alpha}(t) | \Psi_{i\alpha}(t) \rangle}, \quad (4)$$

where \hat{X} is the position operator. In the present study we calculate it only for $i=0$ because the initial state is considered to be located on the atom $i=0$. Also we assume that the atomic-like orbitals are normalized as $\langle \Psi_{i\alpha} | \Psi_{i\alpha} \rangle = 1$.

Substituting Eq.(3) into Eq.(4), one can write

$$\begin{aligned} D_i(t) &= \frac{1}{tN} \sum_{\alpha} \langle i\alpha | e^{i\hat{H}t/\hbar} \hat{X} e^{-i\hat{H}t/\hbar} e^{i\hat{H}t/\hbar} \hat{X} e^{-i\hat{H}t/\hbar} | i\alpha \rangle \\ &= \frac{1}{tN} \sum_{\alpha} \langle i\alpha | \left\{ \hat{X}(t) \right\}^2 | i\alpha \rangle, \end{aligned} \quad (5) \text{ and}$$

where N denotes the number of atomic-like orbitals on a site. In order to express clearly an initial position, Eq.(5) is expressed as

$$D_i(t) = \frac{1}{tN} \sum_{\alpha} \langle i\alpha | \left\{ \hat{X}(t) - \hat{X}(0) \right\}^2 | i\alpha \rangle. \quad (6)$$

Assuming that those atomic-like functions form a complete orthogonal set ($\sum_{j\beta} |j\beta\rangle\langle j\beta| = \hat{\mathbf{1}}$), equation (6) can be rewritten as

$$D_i(t) = \frac{1}{tN} \sum_{j_1\beta_1} \sum_{j_2\beta_2} \sum_{j_3\beta_3} \sum_{j_4\beta_4} \sum_{j_5\beta_5} \left\{ \langle i\alpha | e^{i\hat{H}t/\hbar} | j_1\beta_1 \rangle \right.$$

$$\begin{aligned} &\times \langle j_1\beta_1 | \hat{X} | j_2\beta_2 \rangle \langle j_2\beta_2 | e^{-i\hat{H}t/\hbar} | j_3\beta_3 \rangle - \langle i\alpha | \hat{X} | j_3\beta_3 \rangle \left. \right\} \\ &\times \left\{ \langle j_3\beta_3 | e^{i\hat{H}t/\hbar} | j_4\beta_4 \rangle \langle j_4\beta_4 | \hat{X} | j_5\beta_5 \rangle \langle j_5\beta_5 | e^{-i\hat{H}t/\hbar} | i\alpha \rangle \right. \\ &\left. - \langle j_3\beta_3 | \hat{X} | i\alpha \rangle \right\}. \end{aligned} \quad (7)$$

Here, j 's and β 's also denote indices of atomic position and atomic orbital, respectively. Equation (7) can be reexpressed in matrix form as

$$\mathbf{D}(t) = \frac{1}{tN} \{ \mathbf{A}(-t) \mathbf{X} \mathbf{A}(t) - \mathbf{X} \}^2, \quad (8)$$

where $(j_1\beta_1, j_2\beta_2)$ component of $\mathbf{A}(t)$ is $A(j_1\beta_1, j_2\beta_2) = \langle j_1\beta_1 | e^{-i\hat{H}t/\hbar} | j_2\beta_2 \rangle$, and $(j_1\beta_1, j_2\beta_2)$ component of \mathbf{X} is $X(j_1\beta_1, j_2\beta_2) = \langle j_1\beta_1 | \hat{X} | j_2\beta_2 \rangle$. The relationship between Eq.(7) and Eq.(8) is

$$D_i(t) = \sum_{\alpha} D(i\alpha, i\alpha)(t), \quad (9)$$

where $D(i\alpha, i\alpha)(t)$ is the diagonal element of the matrix $\mathbf{D}(t)$. From Eq.(8) we thus find that the calculation of the electron diffusivity needs only two kinds of matrix, $\mathbf{A}(t)$ and \mathbf{X} .

The time evolution operator $\exp\left(-i\hat{H}t/\hbar\right)$ in Eq.(7) is calculated approximately by the Chebyshev expansion of the first kind. For scalar argument x , the Chebyshev expansion of a function in degree of n is defined as follows:

$$f_n(x) = \sum_{k=0}^{n-1} d_k T_k(x), \quad (10)$$

where

$$d_k = \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n T_k(x_j) f(x_j), \quad (11)$$

$$x_j = \cos \left\{ \frac{(2j-1)\pi}{2n} \right\}. \quad (12)$$

The Chebyshev polynomial of degree n denoted by $T_n(x)$ is given by the explicit formula,

$$T_n(x) = T_n(\cos \theta) = \cos n\theta, \quad (13)$$

therefore, the argument x is restricted to $[-1, 1]$. If original value x' is restricted to $[X_{min}, X_{max}]$, x' should be made a linear transformation as

$$x = \frac{2x' - (X_{max} + X_{min})}{X_{max} - X_{min}}. \quad (14)$$

However, x_j of $f(x_j)$ in Eq.(11) is not restricted to $[-1,1]$. Replacing x_j in Eq.(12) with x'_j , the x'_j of $[X_{min}, X_{max}]$ can be obtained using Eq.(14) as

$$\begin{aligned} x'_j &= \frac{X_{max} - X_{min}}{2} x_j + \frac{X_{max} + X_{min}}{2} \\ &= m_a x_j + m_b. \end{aligned} \quad (15)$$

T_n holds a recurrence relation;

$$\begin{aligned} T_n(x) &= 2xT_{n-1}(x) - T_{n-2}(x), \quad n \geq 2 \\ T_0(x) &= 1, \quad T_1(x) = x. \end{aligned} \quad (16)$$

The time evolution operator can be expanded by the Chebyshev polynomials as

$$\langle j_1 \beta_1 | e^{-i\hat{H}t/\hbar} | j_2 \beta_2 \rangle = \sum_{k=0}^{n-1} d_k(t) \langle j_1 \beta_1 | T_k(\hat{H}) | j_2 \beta_2 \rangle. \quad (17)$$

The Chebyshev polynomials of the Hamiltonian operator are calculated using the recurrence formula Eq.(16) with x replaced by the Hamiltonian operator \hat{H} . We use the atomic unit hereafter (see Appendix A). Equation(10) can be reexpressed using the Bessel function of the first kind. The Bessel function is defined as

$$J_n(z) = \left(\frac{z}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k (z/2)^{2k}}{k! \Gamma(n+k+1)}, \quad (18)$$

$z \neq$ negative real number

where $\Gamma(n)$ is the Gamma function. The Gamma function is defined as

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1} dt, \quad \text{Re}[z] > 0 \quad (19)$$

and, if z is positive integer number, then

$$\Gamma(z) = (z-1)!. \quad (20)$$

In using the Bessel function, we utilize the formulas,

$$\exp(iz \sin \theta) = \sum_{n=-\infty}^{\infty} J_n(z) \exp(in\theta), \quad (21)$$

and

$$J_{-n}(z) = (-1)^n J_n(z). \quad (22)$$

Using these formulas, a function in Eq.(11) can be replaced by

$$\begin{aligned} f(x_j) &= \exp(-ix'_j t) \\ &= \exp(-im_a x_j t - im_b t), \end{aligned} \quad (23)$$

where m_a, m_b are defined in Eq.(15). Equation(23) can be rewritten using Eq.(12) and Eq.(21) as

$$\begin{aligned} \exp(-ix_j t) &= \sum_{n=-\infty}^{\infty} J_n(m_a t) \exp\left\{-i\frac{m\pi}{2n}(2j-1) - i\frac{m\pi}{2}\right\} e^{-im_b t} \\ &= \sum_{n=-\infty}^{\infty} J_n(m_a t) \exp\left\{-i\frac{m\pi}{2n}(2j-1)\right\} \exp\left\{-i\frac{m\pi}{2}\right\} e^{-im_b t} \\ &= \sum_{n=-\infty}^{\infty} J_n(m_a t) \exp\left\{-i\frac{m\pi}{2n}(2j-1)\right\} (-i)^m e^{-im_b t}. \end{aligned} \quad (24)$$

Therefore, substituting Eq.(24) into Eq.(10), one obtains

$$\begin{aligned} f_n(\hat{H}) &= \sum_{m=-\infty}^{\infty} (-i)^m J_m(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n T_k(x_j) \exp\left\{-i\frac{m\pi}{2n}(2j-1)\right\} T_k(\hat{H}) e^{-im_b t} \\ &= J_0(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n T_k(x_j) T_k(\hat{H}) e^{-im_b t} \\ &\quad + \sum_{m=1}^{\infty} (-i)^m J_m(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n T_k(x_j) \exp\left\{-i\frac{m\pi}{2n}(2j-1)\right\} T_k(\hat{H}) e^{-im_b t} \\ &\quad + \sum_{m=1}^{\infty} (-i)^{-m} J_{-m}(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n T_k(x_j) \exp\left\{i\frac{m\pi}{2n}(2j-1)\right\} T_k(\hat{H}) e^{-im_b t}, \end{aligned} \quad (25)$$

and using Eq.(22),

$$\begin{aligned} (-i)^{-m} J_{-m}(m_a t) &= i^m (-1)^m J_m(m_a t) \\ &= (-i)^m J_m(m_a t). \end{aligned} \quad (26)$$

Substituting Eq.(26) into Eq.(25), the time-evolution operator can be expressed as

$$\begin{aligned} \exp(-i\hat{H}t) &= J_0(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n n T_k(x_j) T_k(\hat{H}) e^{-im_b t} \\ &\quad + \sum_{m=1}^{\infty} (-i)^m J_m(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n T_k(x_j) 2 \cos \left\{ \frac{m\pi}{2n} (2j-1) \right\} T_k(\hat{H}) e^{-im_b t} \\ &= J_0(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} \sum_{j=1}^n n T_k(x_j) T_k(\hat{H}) e^{-im_b t} \\ &\quad + \sum_{m=1}^{\infty} (-i)^m J_m(m_a t) \sum_{k=0}^{n-1} \frac{2}{n(1+\delta_{k0})} 2 \sum_{j=1}^n T_k(x_j) T_m(x_j) T_k(\hat{H}) e^{-im_b t}. \end{aligned} \quad (27)$$

The Chebyshev polynomials have a following property:

$$\sum_{j=1}^n T_k(x_j) T_m(x_j) = \begin{cases} \frac{n}{2} & ; k = m \neq 0 \\ n & ; k = m = 0 \\ 0 & ; k \neq m \end{cases}. \quad (28)$$

Finally, the time-evolution operator can be rewritten, using Eq.(27) and Eq.(28), as

$$\begin{aligned} \langle j_1 \beta_1 | \exp(-i\hat{H}t) | j_2 \beta_2 \rangle &= \sum_{m=0}^{\infty} (2 - \delta_{m0}) (-i)^m \\ &\quad \times J_m(m_a t) \langle j_1 \beta_1 | T_m(\hat{H}) | j_2 \beta_2 \rangle e^{-im_b t} \end{aligned} \quad (29)$$

Here we use tight-binding Hamiltonian matrix, thus, after the fashion of Eq.(8), Eq.(29) can be expressed in a matrix form as

$$\mathbf{A}(t) = \sum_{m=0}^{\infty} (2 - \delta_{m0}) (-i)^m J_m(m_a t) T_m(\mathbf{H}) e^{-im_b t}. \quad (30)$$

In the case of $\mathbf{A}(-t)$

$$\mathbf{A}(-t) = \sum_{m=0}^{\infty} (2 - \delta_{m0}) i^m J_m(m_a t) T_m(\mathbf{H}) e^{im_b t}, \quad (31)$$

where \mathbf{H} is the tight-binding matrix (see Appendix B). In similar to Eq.(14), original Hamiltonian matrix \mathbf{H}' can be made a linear transformation as

$$\mathbf{H} = \frac{2\mathbf{H}' - (\lambda_{max} + \lambda_{min})\mathbf{I}}{\lambda_{max} - \lambda_{min}}, \quad \lambda_i \in [\lambda_{min}, \lambda_{max}] \quad (32)$$

where λ_i is the eigenvalue of the \mathbf{H}' . In Eq.(15), X_{min} and X_{max} are replaced by λ_{min} and λ_{max} , respectively. In order to avoid eigenvalue calculation, we use the Gershgorin Circle theorem. This theorem is the following:

Let \mathbf{A} be a square complex matrix. Around every element a_{ii} on the diagonal of the matrix, we draw a circle with radius of the sum of the norms of the other elements on the same row $\sum_{j \neq i} |a_{ij}|$. Such circles are called Gershgorin discs. Every eigenvalue of \mathbf{A} lies in one of these Gershgorin discs. Let λ be an eigenvalue of \mathbf{A} . Then, this theorem can be expressed as

$$|\lambda - a_{ii}| \leq \sum_{j \neq i} |a_{ij}|. \quad (33)$$

We employ the tight-binding representation for the Hamiltonian matrix which includes only the effects of nearest-neighbor interaction. Thus, instead of integrating the expectation value, the mean displacement of electron can be approximated by

$$\begin{aligned} &\sum_{j_1 \beta_1} \sum_{j_2 \beta_2} \langle j_1 \beta_1 | \hat{X} | j_2 \beta_2 \rangle \\ &= \sum_{j_1 \beta_1} \left[\langle j_1 \beta_1 | \hat{X} | j_1 - 1, \beta_1 \rangle + \langle j_1 \beta_1 | \hat{X} | j_1 \beta_1 \rangle \right. \\ &\quad \left. + \langle j_1 \beta_1 | \hat{X} | j_1 + 1, \beta_1 \rangle \right]. \end{aligned} \quad (34)$$

We then assume that integrals have nonzero values only if the two orbitals are of same kind. Integrals for

orbitals on the same atom are approximated as positions of the atom accompanying the orbitals. Similarly, integrals for nearest-neighbor orbitals are approximated as positions of their bond center.

We explained how to obtain the electron diffusivity so far. Hereafter, we explain how to obtain the energy dependent electron diffusivity.

We have to consider the density of states (DOS) in nanostructured semiconductors in order to include the effect of incident electron energy, E , from electrodes. Using spectral density function $\delta(E - \hat{H})$ [18], DOS can be expressed as

$$\rho(E) = \text{Tr} \left[\delta(E - \hat{H}) \right]. \quad (35)$$

Using the orthogonality of the Chebyshev polynomials, the spectral density function can be rewritten as

$$\delta(E - \hat{H}) = \sum_{m=0}^{\infty} \frac{2}{\pi(1 + \delta_{m0})\sqrt{1 - E^2}} T_m(E) T_m(\hat{H}). \quad (36)$$

The energy dependent diffusivity is defined using spectral density function and Eq.(8) in matrix form as

$$\mathbf{D}(E, t) = \frac{\mathbf{D}(t)\mathbf{B}(E)}{\sum_{\alpha} \langle i\alpha | \delta(E - \hat{H}) | i\alpha \rangle}, \quad (37)$$

where $(j_1\beta_1, j_2\beta_2)$ component of $\mathbf{B}(E)$ is $B(j_1\beta_1, j_2\beta_2) = \langle j_1\beta_1 | \delta(E - \hat{H}) | j_2\beta_2 \rangle$. The energy dependent diffusivity value can be obtained like Eq.(9) as

$$D_i(E, t) = \sum_{\alpha} D(i\alpha, i\alpha)(E, t). \quad (38)$$

The diffusivity evolves ballistically in a short-time regime as

$$D_i(E, t) = v^2(E)t, \quad (39)$$

where $v(E)$ is the electron velocity at energy E . Thus, the electron velocity can be obtained from the slope of the diffusivity against time. For calculating mean-free path, we need to estimate the elastic scattering time. The elastic scattering time can be obtained approximately by finding the time when the diffusivity begins to leave from the linearity in the short-time regime. Mean-free path is thereby expressed as

$$l(E) = v(E)\tau, \quad (40)$$

where τ is the elastic scattering time.

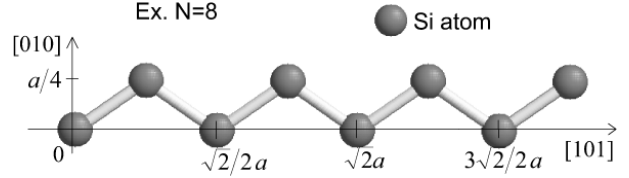


FIG. 1: Semiconductor chain model

3. MODEL

In the previous sections, we have developed basic formalisms for electron dynamics. The theory is now applied to a model system for validation.

The model system we adopted is Si chains shown in Fig.1, where a is chosen to be the bulk value of lattice constant for diamond structure. The principal axis of the chain is equivalent to that along the [101] direction in diamond structure.

4. RESULTS

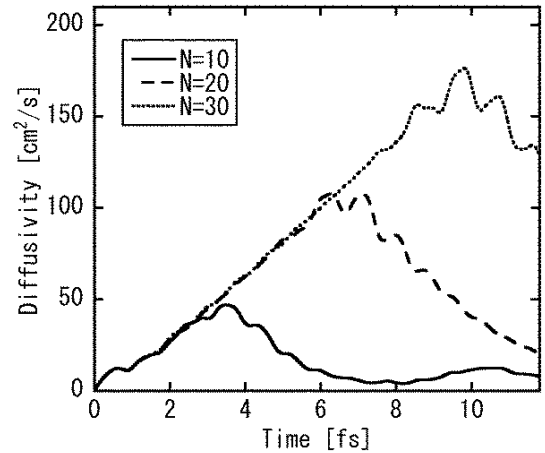


FIG. 2: Diffusivity vs. time for different lengths N . The time scale, in which the diffusivity increases linearly, is getting longer with increase of N .

Figure 2 shows calculated diffusivity for Si chain with lengths $N=10, 20$ and 30 . Diffusivity depends on the initial position i and the initial orbital α . In Fig.2, we show the diffusivity for the electron initially at $i = 1$. The diffusivities increase linearly up to about 2.7fs, 5.5fs and 8.0fs, respectively. Thus, the time scale, in which the diffusivity increases linearly, becomes longer as the length of Si chain increases.

5. CONCLUDING REMARKS

The time scale in which the diffusivity increases linearly corresponds to a ballistic regime of electron motion and the length of ballistic motion is equal to the mean free path of an electron in the system. Consequently, our model shows a ballistic behavior of electrons in Si chains. The decrease of diffusivity after the peak may be due to the interference with the electron reflected at the end of Si chain.

The remaining issues are the following. Although the mean-free path was calculated, relationship between the mean-free path and the DOS has not been understood clearly. Also to compare directly with experiments, we need to evaluate conductance in nanowire with reflectionless electrodes. In order to confirm validity of the theory developed in this paper, we should try to calculate it using the Landauer formula and/or the non-equilibrium Green's function. Our approach is useful to analyze time-dependent electronic behavior and helpful to design nanostructured gates.

APPENDIX

A. Atomic Unit

In the atomic unit, all physical quantities are normalized with the electron mass $m = 1$ [a.u.], the electronic charge $e = 1$ [a.u.], the Plank constant $\hbar = 1$ [a.u.], the Bohr radius $a_B = 1$ [a.u.] $=0.5291772108$ [Å], the energy unit 1 [a.u.] $=27.2113845$ and the time unit 1 [a.u.] $=0.0241888$ [fs].

B. Tight-binding Matrix

Our tight-binding model[19] for Si is based on the paper by I. Kwon *et al.*[20]. The tight-binding parameters are distance-dependent. The atomic interactions are short ranged and decay more rapidly than simple exponentials. The parameters in this model were found by fitting to the phase diagram and energy-volume curves for several polymorphs of crystalline silicon including diamond structure.

The tight-binding matrix element is given by

$$h_\alpha(r) = h_\alpha(r_0) \left(\frac{r_0}{r}\right)^n \times \exp \left\{ n \left(- \left(\frac{r}{r_{c\alpha}}\right)^{n_{c\alpha}} + \left(\frac{r_0}{r_{c\alpha}}\right)^{n_{c\alpha}} \right) \right\}, \quad (41)$$

where α denotes the four tight-binding overlaps. The tight-binding parameters for their best fit are displayed in Table I.

In the case of the system with an impurity atom (Ge), we add the differences from Si atomic-orbital energy to those of Ge [21].

TABLE I: Parameters for the silicon $r_0 = 2.360352\text{\AA}$, $n = 2$, $E_s = -5.25\text{eV}$, $E_p = 1.20\text{eV}$, $E_0 = 8.7393204\text{eV}$

α	$ss\sigma$	$sp\sigma$	$pp\sigma$	$pp\pi$
$h_\alpha(r_0)$ (eV)	-2.038	1.745	2.75	-1.075
$n_{c,\alpha}$	9.5	8.5	7.5	7.5
$r_{c,\alpha}$ (Å)	3.4	3.55	3.7	3.7

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