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Substrate Effects for Atomic Chain Electronics

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A substrate for future atomic chain electronics, where adatoms are placed at designated positions and form atomically precise device components, is studied theoretically. The substrate has to serve as a two-dimensional template for adatom mounting with a reasonable confinement barrier and also provide electronic isolation, preventing unwanted coupling between independent adatom structures. For excellent structural stability, we demand chemical bonding between the adatoms and substrate atoms, but then good electronic isolation may not be guaranteed. Conditions are clarified for good isolation. Because of the chemical bonding, fundamental adatom properties are strongly influenced: a chain with group IV adatoms having two chemical bonds, or a chain with group III adatoms having one chemical bond is semiconducting. Charge transfer from or to the substrate atoms brings about unintentional doping, and the electronic proeprties have to be considered for the entire combination of the adatom and substrate systems even if the adatom modes are well localized at the surface.

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I. Introduction

When the semiconductor device size is reduced to 0.07 μm, the number of dopant atoms in the channel is no longer macroscopic, typically less than a hundred [1-3]. A spatial distribution of these dopant atoms fluctuates statistically from device to device even in identically design and fabricated devices, and this places a serious limitation for integration. It may be possible to control dopant positions to some extent [3], but an ultimate control with atomic precision might be difficult. One fundamental solution to this problem is to create electronics that are atomically precise, ordered, but preferably simple. Atomic chains, which are precise structures of adatoms created on an atomically regulated surface using atom manipulation technology [4], are candidates for constituent components in future electronics. All the adatoms will be placed at designated positions on a substrate, and all the device structures are precise, free from any statistical deviations.

There are two possible schemes to mount adatoms on a substrate surface. For excellent electronic isolation between the adatom and substrate systems, we may want to forbid chemical bonding between the adatoms and substrate atoms, and confine adatoms with a van der Waals potential. For excellent structural stability, we may allow chemical bonding between the adatoms and substrate atoms so that adatoms are not displaced with thermal agitation from their ideal positions. The van der Waals scheme is shown to provide insufficient confinement of adatoms even at low temperatures [5], and may not be appropriate.

In this paper, the chemical bonding scheme is studied in detail. Because of the chemical bonding to the substrate atoms, the electronic isolation between the adatom and substrate systems is not guaranteed. We study the localization conditions of adatom modes at the surface using a one-

dimensional tight-binding model in Sec. II. Chemical bonding influences the fundamental properties of adatoms, such as whether adatom chains are metallic or semiconducting, and this is explained based on a tight-binding picture in Sec. III. The band structure of semiconducting Ge adatom chains realized on a Si (100) surface where unused Si dangling bonds are saturated with H atoms is studied with a self-consistent tight-binding method. Summary is given in Sec. IV.

II. Conditions for Surface Localization and Electronic Isolation

Maximum structural stability is expected for the chemical bonding scheme. Instead, main concern is whether the adatom and substrate systems can be electronically isolated. In the worst scenario, an electron wave function for the adatom modes does not decay but penetrate deep inside the substrate and cannot be distinguished from the bulk modes. This will result in unwanted crosstalk among adatom structures that are designed to be independent. We use a one-dimensional tight-binding model with universal parameters [6] to study the qualitative aspect of the problem. Multi-dimensional models are not quite rewarding since we are interested in how the wave functions decay perpendicular to the substrate surface. In order to see this decay effectively, we need to have many periods, where results are shown to be independent if the number of layers is larger than 10, and this is not easy with multi-dimensional models, although we need to proceed to this direction if a specific combination of adatoms and substrate surfaces is of interest.

Figure 1 shows (a) the energy levels and (b) the electron existence probability at the edge atoms for a chain of 24 Si atoms; (c) and (d) are the same set of plots for a chain of 22 Si atom with a H atoms placed at each edge. They are plotted as a function of the lattice spacing. By changing it from infinity to a finite value as an gedanken experiment [7], it is shown that how edge states, one-dimensional counterparts of surface states having significant amplitude at the edge atoms and

decaying exponentially into the middle of the chain, are created from atomic levels of constituent atoms. We imagine that the substrate is made by bunching a lot of one-dimensional atomic chains. It is our interest to show when these edge states appear, whose wave function has an amplitude mostly on the edge atoms, and decay exponentially deep inside the chain. 3s- and 3p-orbitals, representing symmetric and antisymmetric orbitals in the chain direction, respectively, are taken into account in the chain direction, and other two 3p-orbitals are assumed to be used for chemical bonding with other chains in a realistic three-dimensional substrate. General linear combinations of s- and p-orbitals reflecting more realistic geometry are possible, but the difference can be absorbed in the redefinition of tight-binding parameters. In the unsaturated Si chain in Fig. 1(a), the widths of 3s- and 3p-originated bands become wider as the lattice spacing is reduced. Around 2.7 Å, there is an s-p band crossing, where 3s- and 3p-originated bands cross. For shorter lattice spacing, a new band gap opens, and there appear two edge states, one from the top of the valence band and the other from the bottom of the conduction band. Since they are located inside the band gap, their wave functions have a significant amplitude at the edge atoms as in Fig. 1(b), and decays exponentially inside the chain. These states can be manipulated with H atoms [8]. In the H-saturated chain, the edge states appear in the uncrossed region with longer lattice spacing, and disappear in the crossed region with shorter lattice spacing.

This complimentary behavior can be interpreted intuitively. Figure 2 is a schematic plots of a typical Bloch function envelope near the vacuum boundary. In the unsaturated chain before the s-p crossing in Fig. 2(a), the wave function has a notch at the vacuum boundary and cannot smoothly connect to the vacuum. By tuning the electron energy, we can change the gradient of the wave function, but not its sign, and thus, it is impossible to achieve smooth connection. After the crossing, the smooth connection is possible this time since the wave function has an opposite

gradient at the vacuum boundary in Fig. 2(b). In the H-saturated case, the role of the additional hydrogen cell is to flip the gradient without changing the functional value. This is possible since a H atom has only one relevant orbital, 1s, which is symmetric in the unit cell. Because of this gradient flip, the existence of the edge states is complimentary with respect to the s-p crossing point. The edge states exist before the s-p crossing as in Fig. 2(c) and disappear after the crossing as in Fig. 2(d).

S-p crossing substrates are those made of semiconducting crystals Si, Ge or GaAs, and many metallic substrates. S-p uncrossing substrates are alkali halides, such as KCl or LiF. On an s-p crossing substrate, the dangling bonds are where electrons are localized, and if saturated with H atoms, these states are eliminated. Oppositely on an s-p uncrossing substrate, H-saturated sites are where electrons are localized, and if H atoms are removed, these states are eliminated. For electronic applications, the *absence* of H atoms on an s-p crossing substrate, or the *presence* of H atoms on an uncrossing substrate serves as an device element where electrons are localized.

Figure 3 depicts how the electronic states of an adatom with chemical bonding to substrate atoms arise with a tight-binding picture. There are two ways to obtain a semiconducting chain: (a) use group IV adatoms with two chemical bonds each, or (b) use group III adatoms with one chemical bond each. A group IV adatom has hybridized four sp^3-orbits. On an (100) surface of a diamond-structure crystal, for example, two of the orbitals are used for forming chemical bonds with other two sp^3-orbitals of the substrate atoms. Each pair forms bonding and antibonding bonds, separated by double the covalent energy (typically several eV) [6]. As a result, two electrons from the adatom and two electrons from the substrate atom(s) occupy two bonding bonds completely and create two covalent bonds. Because of the large covalent energy, the bonding bonds have a very low energy and do not contribute to the adatom properties. The remaining two

sp^3-orbitals are then rehybridized and form an sp-orbital and a p-orbital. After the formation of a chain structure, the sp- and p-orbitals will become valence and conduction bands, respectively. The situation is similar for a group III adatom. The only difference is that after the sp^3-hybridization, the atom is rehybridized to have two sp-orbitals and two p-orbitals. One sp-orbital is used for a covalent bond with a substrate atom, and therefore one electron is waisted. The unused sp-orbital forms a valence band, and two orbitals form two conduction bands. Adatom bands can be calculated with a self-consistent tight-binding method based on this picture. With a similar argument, a chain with group II adatoms with no chemical bonds is semiconducting, and this is consistent with the previous results [9].

Although the edge states for a single adatom has an energy level inside the bulk band gap on an s-p crossing substrate as discussed above, the entire adatom bands may not necessarily be included in the bulk band gap. Generally, there may be an overlap with the band gap. From an electronics application point of view, this is not plausible, but the overlap may not be fatal. There has been an experiment observing such surface states and the bulk states in the current-voltage characteristics obtained with scanning tunneling microscopy for Si (111) [10]. The normalized conductance plot as a function of voltage showed five peaks, four attributed to the surface states and one to the bulk states, where the surface peak positions were consistent with a model assuming *unperturbed* surface and bulk states. We can argue that the coupling was so weak that no significant modulation in peak positions resulted, although this did not directly clarify what happened for electronic isolation between the surface and bulk states. In this article, it is assumed that this coupling is small enough, but this isolation problem has to be studied further.

III. Adatom Bands with Self-consistent Tight-binding

We study the band structures of a Ge adatom chain on Si (100), where unused dangling bonds are saturated with H atoms as shown in Fig. 4, where such hydrogenated Si surface is quite stable [11]. According to the tight-binding picture above, this chain is semiconducting, and the wave function is localized at the chain. Because of Ge atomic levels quite close to those of a Si atom, the edge states are localized well inside the bulk Si band gap, and will be a good system to study. In fact, if the adatom has atomic levels quite different from those of substrate atoms, electron localization is weaker when the adatom relevant atomic level has a significant overlap [5]. We note that there are two kinds of adatom chains, σ- and π-chains depending on how the covalent bonds align with respect to the chain direction as in Fig. 4, and the resultant chain properties are significantly different, in spite of exactly the same lattice spacing in both chains.

Atoms are numbered such that adatoms are 0, the nearest neighbors are 1, and the second nearest neighbors are 2, where last two belong to the substrate. Charges are assumed to be distributed up to these second nearest neighbors, and therefore charge neutrality holds inside the unit cell. Charge amount z_i's indicate the number of excess electrons on atom 0, and reflect wave function amplitudes. Thus, they are determined by the tight-binding parameters, diagonal matrix elements ε_i's and off-diagonal matrix elements V's. In turn, these tight-binding parameters are functions of charges z_i's through the Coulomb interaction, and have to be determined self-consistently [12]. As usual, the Coulomb interaction is assumed to change only diagonals from ε_i^{orig}'s, equivalent to atomic term values [6], to ε_i's and not V's. There are six unknowns, ε_0, ε_1, ε_2, z_0, z_1, and z_2. Using a bond-orbital approximation introducing the simplest off-diagonal parametrization [6] and appropriate linearization [12], we express this self-consistency by:

$$z_0 = (\varepsilon_1 - \varepsilon_0)/V_2 \ , \qquad (1)$$

$$z_1 = (\varepsilon_0 - \varepsilon_1)/2V_2 + (\varepsilon_2 - \varepsilon_1)/2V_2' \ , \tag{2}$$

$$z_2 = (\varepsilon_1 - \varepsilon_2)/2V_2' \ , \tag{3}$$

$$\varepsilon_i = \varepsilon_i^{\text{orig}} + c_{i0}z_0 + c_{i1}z_1 + c_{i2}z_2 \ , \quad (i = 0, 1, \& \ 2) \ , \tag{4}$$

Equations (1) - (3) show how the tight-binding parameters determine the charges (wave functions), where V_2 is an off-diagonal element, the covalent energy for atoms 0 and 1, and V_2' is the same for atoms 1 and 2. A charge conservation relation of $z_0 + 2z_1 + 2z_2 = 0$ automatically holds in this formalism. Equations (4) show how the charges modify the diagonal tight-binding parameters. c_{ij} stands for a coefficient of the Coulomb interaction for atom i due to charge z_j. Coulomb interaction is due to intra-atomic (self-charging) repulsion, inter-atomic repulsion from the same unit cell, and Madelung interaction from the other unit cells. The Madelung energies are evaluated numerically and expressed as a function of only z_1 and z_2 using the charge conservation relation. They are normalized to $W = e^2/3.84$. Each c_{ij} is given by

$$c_{00} = U_0 \ ,$$

$$c_{01} = 2e^2/2.35 - 0.732W \ ,$$

$$c_{02} = 2e^2/3.17 - 1.17W \ ,$$

$$c_{10} = e^2/2.35 \ ,$$

$$c_{11} = U_1 + e^2/3.84 - 0.00644W \ ,$$

$$c_{12} = e^2/5.12 + e^2/1.48 - 1.05W \ ,$$

$$c_{20} = e^2/3.17 \ ,$$

$$c_{21} = e^2/5.12 + e^2/1.48 - 0.177W ,$$

$$c_{22} = U_2 + e^2/6.26 - 0.382W , \qquad (5)$$

where U_i is a self-charging energy for atom i. For example, c_{00} corresponds to a Coulomb energy shift for atom 0 due to its own charge, represented by the intra-atomic repulsion U_0. c_{01} corresponds to the shift for atom 0 due to neighboring charges z_1's that are 2.35 Å apart from atom 0 in the same unit cell (interatomic repulsion $e^2/2.35$ x 2) and due to charges z_1 in the other unit cells (Madelung energy -0.732W). Other coefficients are derived similarly. Necessary tight-binding parameters for H including the intra-atomic repulsion energy are taken from Ref. 13 and others for Ge and Si are taken from Ref. 12. Once all the constants are determined, numerical solution is easy after a routine matrix inversion. A similar procedure applies to the π-chain.

It should be noted that in the present formalism, we do not have any quantity corresponding to a chemical potential. We may tend to think that electrons will flow from an atom with a higher occupied level to an atom with a lower occupied level, and a certain quantity (chemical potential) becomes the same over the entire system in equilibrium. Diagonal elements ε_i's do not play the role of this chemical potential. Indeed electrons do flow from a higher-occupied-level atom to a lower-occupied-level atom, but the flow stops before the diagonal elements become equal. This is clearly seen in the Eqs. (1) - (3), where the difference in ε_i's supports nonzero charges.

Once the charges are calculated, it is straightforward to obtain the band structures with a tight-binding method. Charges do not change the band shape, but shift the entire adatom bands upwards if adatoms are negatively charged, or downwards if positively charged. This shift changes the position of the Fermi energy, and hence semiconductor chains are unintentionally

doped because of this charge transfer.

The band structure for σ-chain is given by

$$\varepsilon(k) = \{\varepsilon_a + \varepsilon_b \pm [(\varepsilon_a - \varepsilon_b)^2 + 8V_{sp\sigma}{}^2 \sin^2 kd]^{1/2}\}/2 \ , \qquad (6)$$

where the lower and upper signs corresponds to the valence and conduction bands, respectively. d is the adatom lattice spacing equal to 3.84 Å, and k is the momentum along the chain. $V_{ll'm}$ is an off-diagonal element between orbitals l and l' (either s or p) for m-bonding (either σ or π), and are generally expressed with universal parameters in the form proportionate to d^{-2} [6]. ε_a and ε_b are defined by

$$\varepsilon_a = (\varepsilon_s + \varepsilon_p)/2 - (|V_{ss\sigma}| + |V_{pp\pi}|) \cos kd \ ,$$
$$\varepsilon_b = \varepsilon_p + 2|V_{pp\sigma}| \cos kd \ . \qquad (7)$$

In the above, ε_s and ε_p are *modified* diagonal matrix elements for s- and p-levels for adatom *after* self-consistent distribution of charges and the modification is calculated with Eq. (4), while $V_{ll'm}$ is independent of them. The valence and conduction bands for π-band are given, respectively, by

$$\varepsilon_v(k) = (\varepsilon_s + \varepsilon_p)/2 - (|V_{ss\sigma}| + |V_{pp\pi}|) \cos kd \ ,$$
$$\varepsilon_c(k) = \varepsilon_p - 2|V_{pp\sigma}| \cos kd \ . \qquad (8)$$

An inserted table in Fig. 5 summarizes the calculated charge transfer, z_0, z_1, and z_2. They are

quite small because of the electronic similarity between Ge and Si atoms, and the linearization in deriving Eqs. (1) - (3) has been justified. Electrons are transferred from the Ge-chain to the substrate atoms (thus unintentional p-doping), and the shifts are - 0.745 eV (z_0 = -0.0124e) and - 0.0552 eV (-0.00626e) for σ- and π-chain, respectively, with e being the unit charge. The shift is larger in the σ-chain than in the π-chain. This is because the second nearest neighbor is H and Si, respectively, where a H atom can absorb electrons more effectively than a Si atom, due to a deeper H 1s-level than a Si 3p-level. Since a C 2p-level is deeper than a Si 3p-level, the opposite situation arises for C adatom chains. Electrons flow from the Si substrate atoms to the C adatoms, resulting in n-doping. Because of these unintentional dopings, the electron filling is a little off from the exact half-integers, and this makes the Peierls or Mott transitions [14] irrelevant.

Figure 5 shows the band structures for σ- and π-chains. As is obvious in the plot, the σ-chain has a typical band structure made of symmetric and antisymmetric orbitals, sp- and p-orbitals, respectively, in the unit cell: the conduction band maximum and the valence band minimum occur at Γ and the conduction band minimum and the valence band maximum occur at the band edge X. This has been already apparent in Eq. (5). The π-chain has two independent π-bands made of two symmetric orbitals, sp and p. Note that the p-orbital is perpendicular to the chain as in Fig. 5, and therefore symmetric in the π-chain, in contrast to the asymmetric p-orbital in the σ-chain. Therefore, the band minimum occur at Γ and the maximum at X for both π-bands. The entire structures for s- and p-chains range around several eV, much wider than the bulk Si band gap. As discussed above this does not immediately mean poor isolation between the surface and bulk modes, and probably is not a serious problem, but expected effects need to be studied in the future.

IV. Summary

The substrate effects on the electronic properties of adatom structures are considered. When the adatoms form chemical bonding to the substrate atoms, some electrons are exclusively used for covalent bonding, and only the remaining electrons can determine the adatom properties. Therefore, chain structures with group IV adatoms having two chemical bonds each to the substrate atoms, or group III adatoms having one chemical bond, are candidate for semiconductors.

A main concern for this chemical bonding scheme is that the electron wave function may not be localized in an adatom structure, but penetrate deep into the substrate. This is the case with s-p uncrossing substrate such as alkali halide crystals. Adatom states are localized at the surface if the substrate is s-p crossing such as many semiconducting and metallic crystals. On an s-p crossing substrate, we can eliminate unwanted surface states by saturation with H atoms, where elimination of dangling bonds means elimination of surface states (complimentary situation on an uncrossing substrate). Ge adatom chains are studied using a self-consistent tight-binding method, and it is shown that two different kinds of chains are possible, σ- and π-chains, depending on the geometrical relation between the covalent bonds and the chain direction.

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Figure Captions

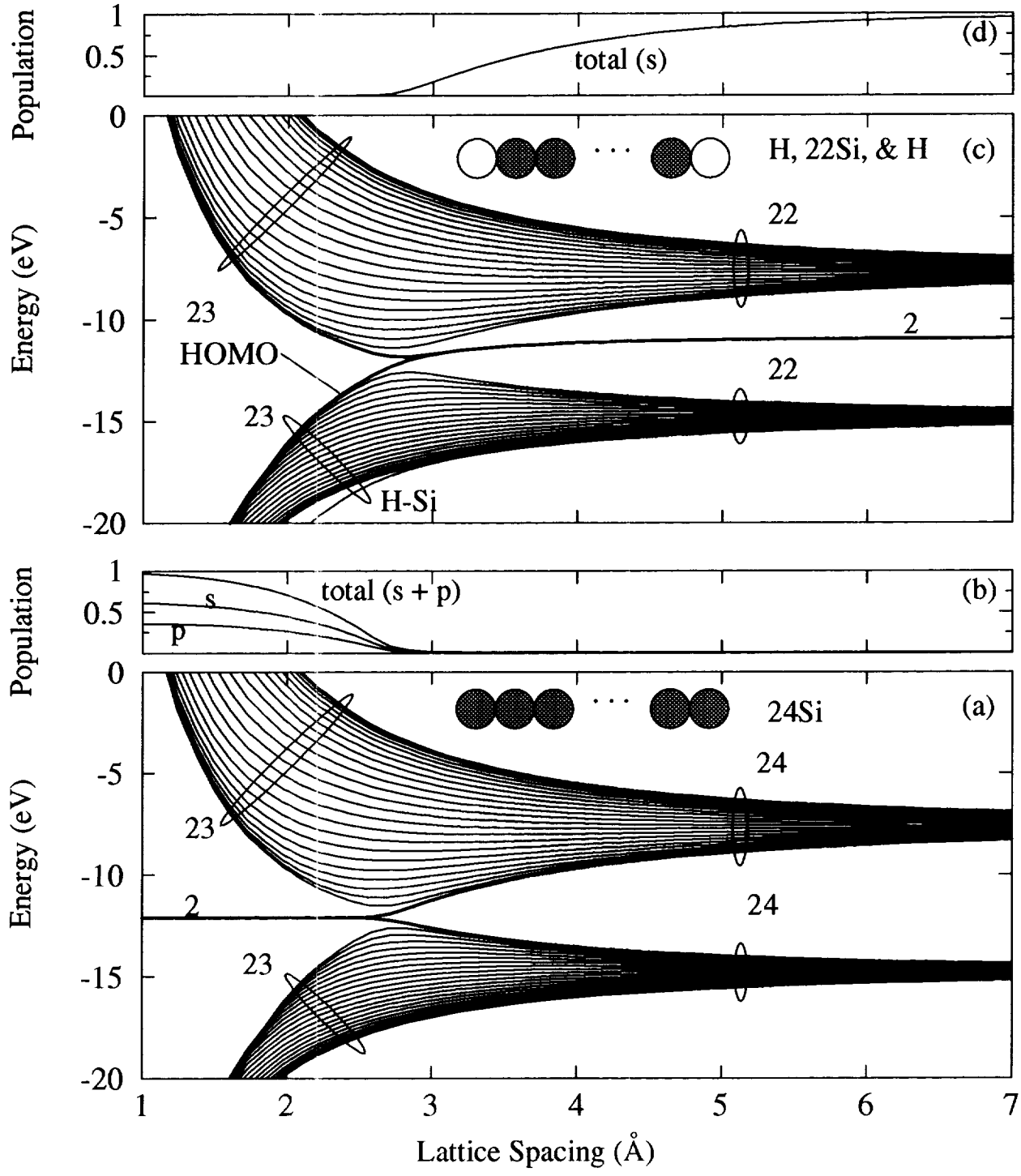
FIG. 1. Edge states as a function of lattice spacing: (a) energy levels and (b) population at edge atoms for band gap modes (thick line) in 24 Si chain; (c) and (d) the same plots in 22 Si chain with two edge H atoms.

FIG. 2. Bloch functions at vauum boundary: for unsaturated chain, (a) long lattice spacing without edge states and (b) short lattice spacing with edge state; for H-saturated chain, (c) long lattice spacing with edge states and (d) short lattice spacing without edge states.

FIG. 3. Tight-binding view for semiconducting adatom chains in the chemical-bonding scheme: (a) group IV adatom with two chemical bonds and (b) group III adatom with one chemical bond.

FIG. 4. Adatom σ- and π-chains on hydrogenated Si(100) surface with adatom charge z_0, nearest neighbor charge z_1, and second nearest neighbor charge z_2.

FIG. 5. Adatom band structures of σ- and π-chains with Ge adatoms on hydrogenated Si(100) surface.


Population
1
0.5
(d)
total (s)
0
-5
-10
-15
-20
Energy (eV)
H, 22Si, & H
(c)
22
23
2
HOMO
22
23
H-Si
Population
1
0.5
s
p
total (s + p)
(b)
0
-5
-10
-15
-20
Energy (eV)
24Si
(a)
24
23
2
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23
1
2
3
4
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6
7
Lattice Spacing (Å)

Fig. 1

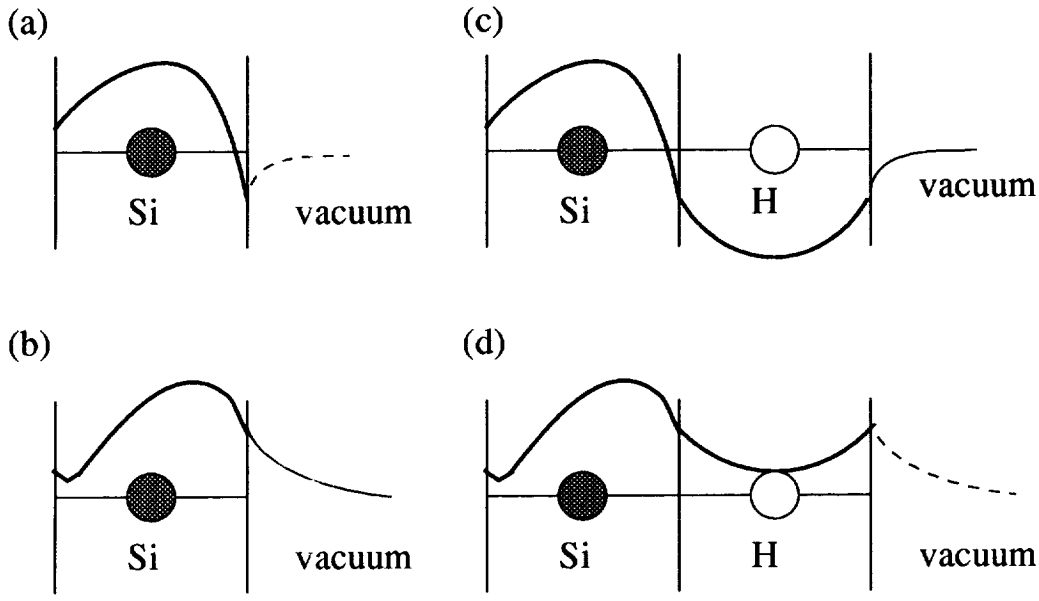
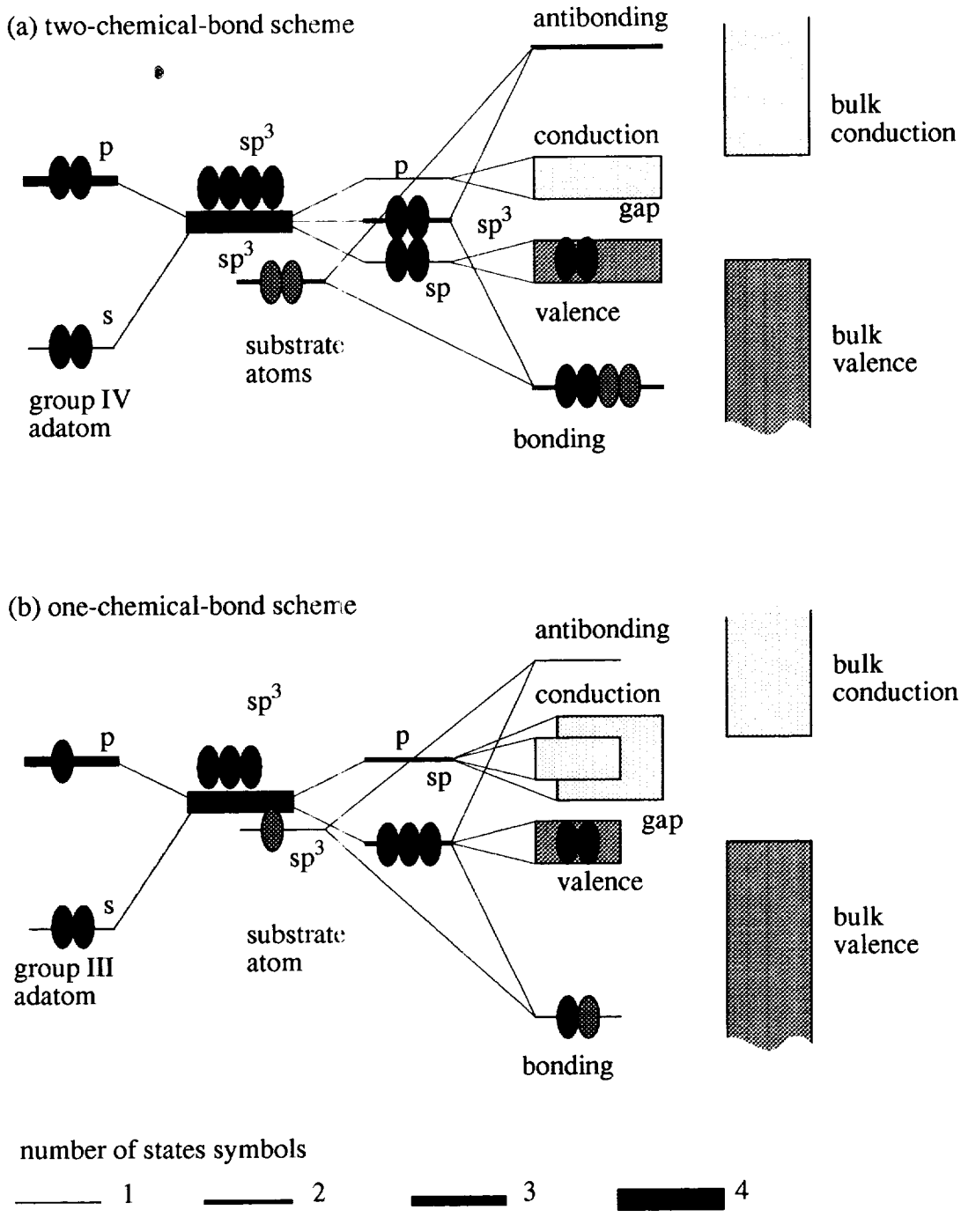


Fig. 2


(a) two-chemical-bond scheme
antibonding
conduction
gap
valence
bonding
p
sp3
sp3
s
p
sp3
sp
substrate
atoms
group IV
adatom
bulk
conduction
bulk
valence
(b) one-chemical-bond scheme
antibonding
conduction
gap
valence
bonding
sp3
p
s
sp3
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valence
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2
3
4

Fig. 3

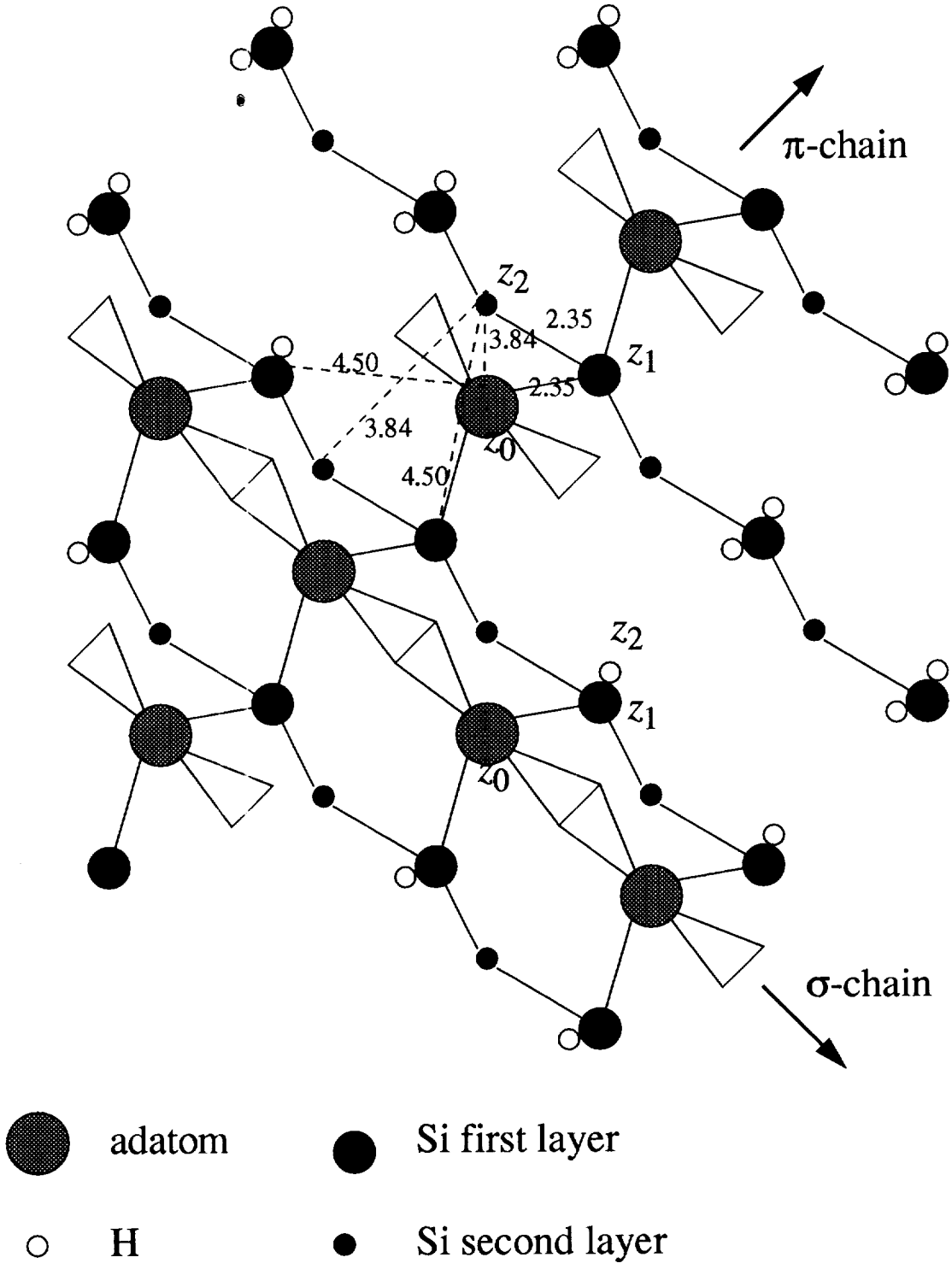
π-chain
σ-chain
z_2
z_1
z_0
2.35
3.84
4.50
2.35
3.84
4.50
z_2
z_1
z_0
adatom
Si first layer
H
Si second layer

Fig. 4

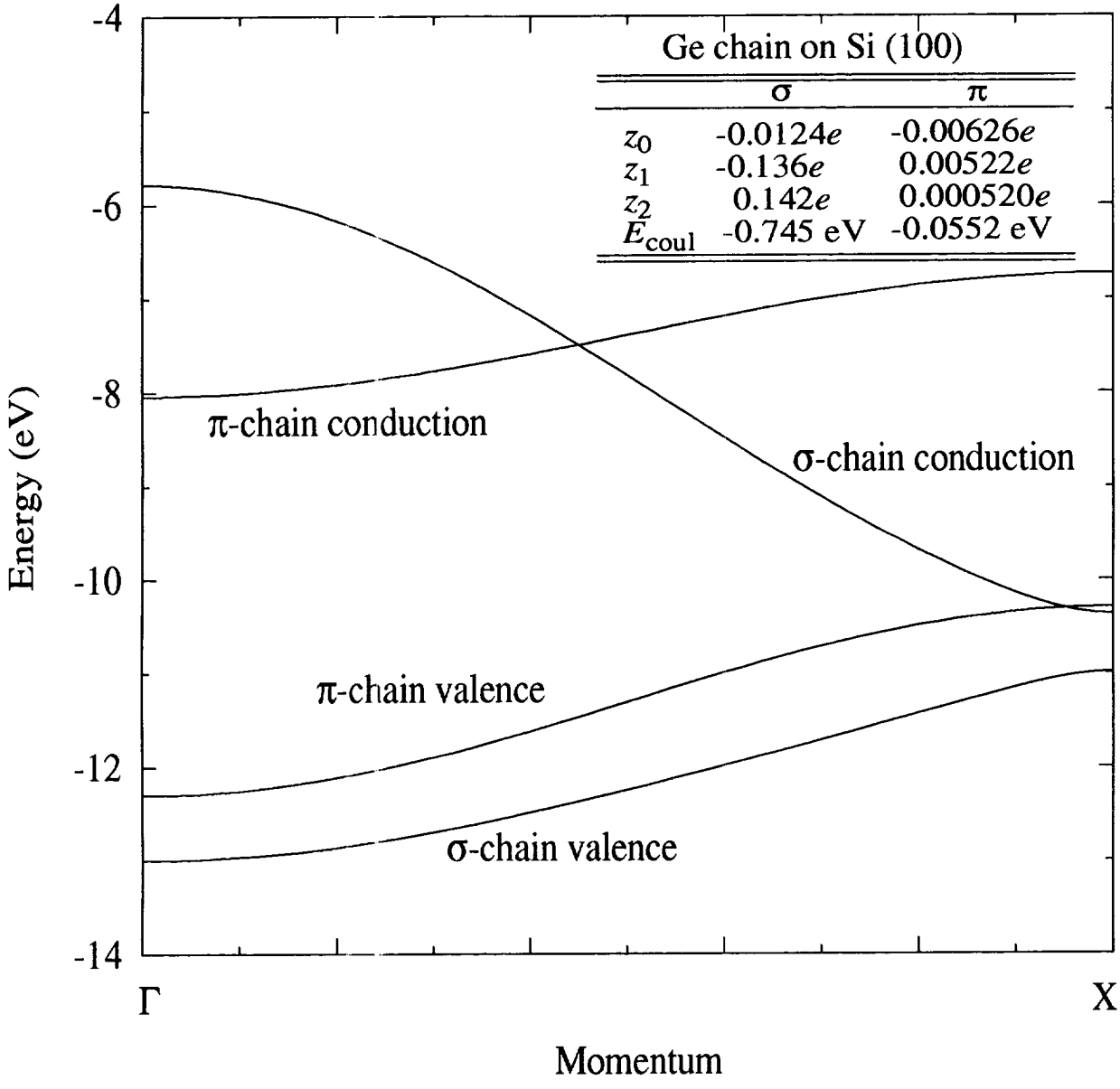
Ge chain on Si (100)
σ π
z_0 -0.0124e -0.00626e
z_1 -0.136e 0.00522e
z_2 0.142e 0.000520e
E_{coul} -0.745 eV -0.0552 eV
π-chain conduction
σ-chain conduction
π-chain valence
σ-chain valence
Energy (eV)
-4
-6
-8
-10
-12
-14
Γ
X
Momentum

Fig. 5