Electron transport through dangling-bond silicon wires on H-passivated Si(100)

Mikaël Kepenekian¹, Frederico D Novaes¹, Roberto Robles¹, Serge Monturet², Hiroyo Kawai³, Christian Joachim²,³ and Nicolás Lorente¹

¹ Centro de Investigación en Nanociencia y Nanotecnología (CSIC-ICN), Campus de la UAB, E-08193 Bellaterra, Spain
² Centre d’Elaboration des Matériaux et d’Etudes Structurales (CEMES), CNRS, 29 rue J. Marvig, F-31055 Toulouse Cedex, France
³ Institute of Materials Research and Engineering, 3 Research Link, Singapore 117602, Singapore

E-mail: mikael.kepenekian@cin2.es

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Abstract

We compute the electron transmission through different types of dangling-bond wire on Si(100)–H (2 × 1). Recent progress in the construction of atomic-size interconnects (Weber et al 2012 Science 335 64) shows the possibility to achieve atomic-size circuits via atomic-size wires using silicon surfaces. Hence, electron transport through quasi-1D Si-based structures is a compelling reality. Prior to these achievements, wires formed by controlled desorption of passivating H atoms off the monohydride Si(100) surface have been shown to be subject to 1D correlations and instabilities (Hitosugi et al 1999 Phys. Rev. Lett. 82 4034). The present calculations are based on density functional theory and evaluate the electron transmission though the minimum-energy 1D structures that can be formed when creating dangling-bonds on Si(100)-(2 × 1)-H. The purpose of this study is twofold: (i) to assess the transport properties of these atomic-size wires in the presence of 1D instabilities; (ii) to provide a fingerprint for experimental identification of the instability through the transport characteristics of the wires. To these aims, we evaluate the electron transport through the wires in the absence of instabilities, in the presence of distortions (Jahn–Teller instabilities) and in the presence of magnetic instabilities (ferro- and antiferro-ordering). We find that instabilities substantially reduce the transport capabilities of dangling-bond wires leading to transmissions that vary so differently with electron energy that an unambiguous identification of the wire type should be accessible in transport experiments.

(Some figures may appear in colour only in the online journal)

1. Introduction

The continuous miniaturization of electronic devices is now reaching the atomic scale. One challenge is to design atomic scale circuits where a single molecule and/or an atomic logic gate can be (i) electronically addressed and (ii) interconnected together by high-conductance wiring [1–4]. Recently, successful attempts have permitted the construction of nanoscale interconnecting structures using silicon as the base material, either by using P dopants [3, 4] or by growing endotaxial Si nanolines on Si surfaces [5]. Previous attempts to construct 1-D-like atomic interconnects were based on the Si(100)-(2 × 1)-H surface, where an aligned row of Si dangling-bonds (DBs) was created by desorbing...
Figure 1. The atomic structure of (a) the Si(100)-(2 × 1)-H surface, (b) the infinite ideal wire drawn along the y direction. H atoms are depicted in cyan, while Si atoms are depicted in red (surface dimers), yellow (others) and blue when holding a dangling-bond.

The existence of DLs on different Si surfaces and facets has been shown to yield very interesting transport properties [17--20]. The transport electronic properties of such wires have been inspected by extended Hückel calculations and explained using a tight-binding model [17, 20]. However, transport calculations in the presence of realistic instabilities of the wires are not available. These calculations are of special importance for a precise electronic-band engineering of DB wires and, eventually, to anticipate the design of surface-based atomic devices adapted to realistic DB wires.

This paper aims at understanding and characterizing electronic transport in the different possible DB wires of desorbed rows of Si(100)-(2 × 1)-H, see figure 1. This paper is then a first account of transport in realistic DB wires together with a transport-based characterization of the wires that can eventually determine their nature via transport experiments.

The transport calculations are performed using the non-equilibrium Green’s function (NEGF) and density functional theory (DFT). In order to complete the first electron transport model proposed by Kawai et al [20], for wires in the absence of instabilities, we study the corresponding infinite ideal wire by means of DFT-based calculations and maximally localized Wannier functions (MLWFs) [21]. This strategy furnishes us with a tight-binding model of DFT quality allowing us to gather extra insight into the main ingredients of transport in DB wires. We follow this study by a complete exploration of different wires under different instabilities. One of our main results is that the computed transmissions are so different that an unambiguous identification of the wire type is experimentally accessible through transport measurements.
2. Computational details

The first-principles calculations are based on density functional theory (DFT) as implemented in SIESTA [22, 23]. Calculations were carried out with the GGA functional in the PBE form [24], Troullier–Martins pseudopotentials [25] and a basis set of finite-range numerical pseudoatomic orbitals for the valence wavefunctions [26].

The structures were relaxed using double-ζ polarized (DZP) basis sets [26]. This level of description has been proven to provide an accurate structural description for silicon-based materials [22]. It has also shown an excellent agreement with plane-wave-based calculations in a previous study on DB wires on Si(100) [16]. The surfaces were modeled using a slab geometry with eight silicon layers and the (4×8) unit cell shown in figure 4. The electronic structure was converged using a 5×3×1 k-point sampling of the Brillouin zone.

The conductance was computed from first-principles, using a single-ζ polarized (SZP) basis set, by means of the TRANSIESTA method [27], within the non-equilibrium Green’s function (NEGF) formalism. The reduction from DZP to SZP basis sets for transport calculations is a common procedure. Brandbyge et al [27] showed that no improvement of the transmission function is obtained when going from SZP to DZP. Moreover, a comparison of a plane-wave calculation of a transmission function with an SZP calculation [28] shows no difference even in the tunneling regime within the spatial extension of the SZP functions. Nevertheless, we inspected the effect of the use of an SZP instead of a DZP basis set (see figure 2). No difference could be observed in the wire’s electron transmission, except for the modification of the bulk gap that is not playing any role in the transmission properties of the DB wires.

In order to reach a better understanding of the transport properties of the DB silicon wires, subsequent transformation of the Kohn–Sham orbitals to maximally localized Wannier functions (MLWFs) [21] was applied. This scheme allows one to obtain localized orthogonal basis sets. As a consequence, MLWFs offer an extremely convenient way to translate the problem in terms of an orthogonal tight-binding approach. Moreover, an ab initio evaluation of the on-site energies and hopping integrals becomes available. The numerical calculations of MLWFs were run with the WANNIER90 code [29], used as a post-processing tool of SIESTA. The interface between both codes was developed earlier by Korytář et al [30, 31].

3. Ideal wire and H-junctions

The fully hydrogenated Si(100) surface presents a (2×1) reconstruction with dimer rows formed along the y (i.e. [110]) direction (see figure 1(a)). Starting from this fully passivated surface, one can construct a DB wire by removing H atoms with an STM tip, along the dimer-row direction (see figure 1(b)). Theoretically, the DB wire obtained without permitting magnetic solutions or geometrical buckling of DB pairs has a metallic character. However, this ‘ideal’ structure is not the minimum-energy conformation of the DB wire [16]. It is nevertheless interesting to understand the transmission properties of this DB wire because it will be our basis to discuss the transmission of realistic wires.

Figure 3 shows the electronic transmission through an infinite ideal wire. As expected from its band structure (see figure 7), the transmission exhibits clear steps featuring the existence of two channels between 0.08 and 0.26 eV above the Fermi energy (E_F), with only one remaining channel for E−E_F taken between −0.53 and 0.08 eV. This result slightly differs from the one previously obtained by Kawai et al [20] from extended Hückel calculations, where the energy range of the one-channel location is as large as the two-channel one (∼0.4 eV), the total non-zero transmission in the surface gap being the same in both calculations.

The intuitive picture is that a transmission through such a non-relaxed DB wire arises from the direct through space coupling between DBs. However, the substrate is thought to play an important role in the transport [20], and a convenient way to remove the direct coupling is to passivate one of the...
Indeed, this specific junction removes only one of the channels and does not affect the second channel (active between 0.08 and 0.26 eV).

At this point, the DFT treatment, although powerful, is too global to give a clear picture of the transport mechanism through surface DB wires and H-junctions. In this regard, the parametrized tight-binding method constitutes an elegant way to model the physics of transport. Thus, one needs to take the best of both worlds and associate the accuracy of DFT-based calculations with the clarity of a simple tight-binding basis set. This is made possible by the use of Wannier functions, which allow one to (i) identify the main couplings, (ii) extract ab initio evaluations of on-site energies and hopping integrals, and (iii) use them in a tight-binding calculation.

4. Wannier function analysis

There is a large freedom in the choice of the Wannier functions used to describe the DB wire, in the sense that they are built to describe a certain energy interval of the band structure of the DB wire, and, also, the points in space around which they will be localized have to be specified as an input for the algorithm. In a first step, we choose to assign one MLWF at each bond and one function per DB along the wire. The chosen energy interval was \(-12 < E - E_F < 3\) eV. A subset of the MLWFs obtained for the ideal DB wire is depicted in figure 6.

With the corresponding Hamiltonian (written in this MLWF basis set), we can study the main electronic couplings in order to rationalize the electronic properties of the DB wire. One important feature is that the direct through space electronic coupling between nearest neighbor DBs is extremely low, \(-0.06\) eV, as compared to the coupling between a DB and its subsurface functions that can reach \(-1.70\) eV. Hence, one cannot interpret this transmission as occurring via a direct through space electron transfer mechanism between DBs since the substrate electronic transport channels dominate along the wire.

From these functions, one can interpolate the band structure. The agreement with the DFT-based band structure is excellent. Regarding the transport properties, we are mainly interested in the metallic band that appears at the Fermi energy resulting from the presence of the DBs. Projections of the metallic band on different sets of MLWFs are depicted in figure 7. Here, the metallic band is correctly described when a large set of subsurface basis functions is included. This indicates that the price to pay for using bond-like orbitals is that a larger number of them is required in order to properly model the transport properties of non-relaxed DBs, i.e. to describe the metallic band accurately.

Another strategy consists in focusing only on the description of the metallic band. Only one basis function is required per DB and the energy window is restricted to the domain of the metallic band. This leads to the calculation of an ‘effective’ orbital (see figure 8) that spreads over the DB and the substrate. As a result, we can reach a 1-D tight-binding description of the system where each site averages the contribution of DBs and subsurface functions.
Figure 6. Plot of dangling-bond-like (left), and subsurface (right) maximally localized Wannier functions. These MLWFs are obtained by assigning one center per bond and allow one to recover the whole band structure of the system.

Figure 7. The interpolated metallic band of the ideal wire along the direction of the DB wire. The color stands for the overlap of the eigenstate with the MLWF corresponding to (a) the dangling-bonds and (b) the dangling-bonds with eight subsurface functions (see figure 6). The Fermi level lies at $-4.25$ eV. The DBs alone cannot account for the whole metallic band. Indeed, the band is well described only when taking into account eight other functions.

Figure 8. Plot of the ‘effective’ MLWF. This MLWF is obtained by assigning only one center per DB and by describing only the metallic band. It can be seen as a weighed ‘mix’ between the functions depicted in figure 6.

The metallic band can then be computed from the MLWF Hamiltonian, improving the calculations by including couplings to two, three or more neighbors. We found that the coupling with the fifth neighbor had to be included in the calculation in order to obtain a quantitative agreement with the DFT-based result.

5. Modeling electron scattering off a single H-junction

As presented earlier (see figure 3), a single H-junction has a transmission of $\sim 1$ in the energy window where it used to be $T(E) = 2$ without any H atom. Furthermore, it quickly drops to values close to zero for lower energies. To model the presence of a saturated DB which acts as a scattering center, the scattering states [32, 33] will be studied, where the asymptotic states are the Bloch states of a periodic DB wire. We will compare the \textit{ab initio} transmission eigenchannels with the solutions found using the ‘effective’ orbital (see figure 8).

We start by characterizing the available asymptotic (Bloch) states at each energy. Figure 9 shows the band structure with the corresponding right- and left-going states. They are labeled channels 1 and 2 respectively in the
Figure 9. The band structure of the ideal DB wire along the direction of the wire for positive and negative values of $k$. Right- and left-going modes are indicated. Above the blue (dashed–double dotted) line there are two modes (channels) that give a maximum transmission of two, and below it only one. $a$ is the distance between two DBs.

following. It can be seen that depending on the energy window, there are two or just one channel. When visualizing these states, the change of the phase for the effective orbital, at each site, is determined by the corresponding $k$ value of the channel.

We move on now to the scattering states. For ideal wires without any scattering center, the scattering states will correspond to the Bloch states at each energy (see figure 10). Both channels 1 and 2 show the expected phase modulation corresponding to $k$ vectors with values of $k_1 \sim -\pi/(2a)$ and $k_2 \sim 0$ (where $a$ is the distance between two DBs).

In the presence of a H atom (saturated DB), the incoming states are scattered as shown in figure 11. For energy values with just one channel and for a left incoming state, the resulting scattering state is a superposition of the incoming wave (characterized by a certain $k_{\text{inc}}$) and the reflected wave (with $k = -k_{\text{inc}}$) weighed by the (complex) coefficient $r$; to the right of the scatterer, the transmitted wave has $k = k_{\text{inc}}$ and is weighed by the transmission coefficient $t$. As an example, in the case of the scattering state at $E - E_F = 0$ (see figure 10(c)), for a right-going state coming from the left, $k_{\text{inc}} \sim -\pi/(2a)$ and $T \sim 0.1$. The transmitted wave corresponds to an outgoing wave with an associated $k \sim -\pi/(2a)$. Since the transmission is low, with $r \sim 1$, the imaginary parts of the incoming and reflected waves cancel, leaving only the real parts of the amplitudes.

The visualization process gets more complicated in the energy window where there are two channels, since now the scattering can couple the two channels (see figure 11). Although the transmission and reflection coefficients could be explicitly obtained from first-principles, we can now use the one-dimensional character of the problem and model the system as a one-dimensional chain, as explained above, using the parameters extracted from the MLWF transformation. This strategy allows us to (i) explicitly obtain the transmission and reflection coefficients and hence the total transmission coefficient $T(E)$ (which depends also on the group velocities), and (ii) obtain the transmission function in less than a second—instead of hours, the typical time it takes to obtain the $T(E)$ from first-principles for the geometries considered here. This latter aspect is particularly important in the case of more complex arrangements involving more than one saturated DB in extended tunnel H-junctions.

The saturated DB is modeled as a defect, in the sense that, at the saturated site, there is no available orbital for the electrons to be transferred through, as depicted in figure 12. Different strategies can be used in order to solve the scattering problem. Here, we have used the multiband quantum transmitting boundary method proposed by Liang et al [34].

When modeling the changes in the tight-binding matrix elements due to the presence of the H atom, one can expect
Bloch waves of different \( k \) scattering defect that effectively mixes the two incoming and shows excellent agreement with the \textit{ab initio} table 1. The corresponding transmission curve is computed similar to the one applied to an ideal DB wire, and given in indicated in figure 12 are obtained from an MLWF treatment and one-dimensional model chain with one saturated DB (sites 1 interaction reduced. Figure 12 shows the scheme of the couplings between the two DBs separated by the saturated that the most affected matrix elements are the electronic transport in these systems: Bloch waves made up scattering properties leaves us with a physical picture for the DB wires.

Figure 12. The one-dimensional model for the DB wires. Site 0 represents a saturated DB, modeled as a defect, i.e. no transfer is possible through this site. The other sites correspond to ‘effective’ orbitals (see figure 8). With respect to the ideal DB wire, the Hamiltonian matrix element that is most affected is the one represented here by \( \beta \), followed by \( \alpha \) (onsite), and \( \beta' \), \( \beta \) and \( \beta' \) do not represent direct hopping between DBs but stand for transfers through the substrate.

Table 1. The MLWF Hamiltonian matrix parameters that were changed when going from the ideal wire to a wire with one saturated DB (together with the introduction of a defect). All the values are given in eV and correspond to the transfer integral matrix element shown in figure 12.

| Chain type | \( \beta \)  | \( \alpha \)  | \( \beta' \)  |
|------------|-------------|-------------|-------------|
| Ideal      | -0.053      | -4.333      | 0.190       |
| 1H         | -0.041      | -4.298      | 0.182       |

that the most affected matrix elements are the electronic couplings between the two DBs separated by the saturated DB, in the sense of having their effective through bond interaction reduced. Figure 12 shows the scheme of the one-dimensional model chain with one saturated DB (sites 1 and \( -1 \) are separated by a saturated DB). The matrix elements indicated in figure 12 are obtained from an MLWF treatment similar to the one applied to an ideal DB wire, and given in table 1. The corresponding transmission curve is computed and shows excellent agreement with the \textit{ab initio} result. Also, for the energy window where there are two channels, the decomposition of the transmission function in terms of the contribution of the scattering of each channel into each other channel shows that they tend to be equally scattered.

The effect of the passivation of one DB is then to create a scattering defect that effectively mixes the two incoming Bloch waves of different \( k \) values. This first inspection of the scattering properties leaves us with a physical picture for the electronic transport in these systems: Bloch waves made up by the effective orbital, which are scattered by a saturated DB as a defect in a linear chain. Due the long range electronic interactions through the substrate, this one-dimensional chain has a somewhat unusual band structure, such that there can be two channels for certain energies that correspond to two Bloch states associated to two different \( k \) values. This degeneracy gives rise to interesting scattering properties.

6. Dangling-bond wires

As previously stated, an ideal finite DB wire relaxes by performing either a Jahn–Teller distortion (NM wire) or a spin polarization with the DBs coupled ferro- or antiferromagnetically (FM and AFM wires). The structures and the energetics of these different atomic surface structures have been previously described [14, 16]. In the case of short DB wires, the AFM state is the most stable. However, the calculated energy difference between AFM and NM or FM configurations remains too small to ignore [14, 16]. Therefore, in this section, the transport properties of the three NM, AFM and FM DB wire configurations are discussed.

The system is divided into left and right leads and a central scattering region, in our case the different possible wires (ideal, NM, AFM and FM) [27, 35]. The self-consistent density matrix is converged in the scattering region, using the open boundary conditions imposed by the leads through their self-energies, using the now standard Green’s function-based method [27]. In order to avoid the sensitive problem of the description of the interface between realistic electrodes and the DB wires, we choose to take advantage of the metallic behavior of the ideal wire (see section 3) and use it as the source of electrons to be transferred through the scattering region. Thus, in our calculations, the roles of the right and left leads are performed by semi-infinite ideal wires. This approximation is necessary given the great complexity of the metal–silicon interface for the simulation of realistic electrodes. Recent experiments have achieved metallic electrodes in silicon [3] by selective doping of extensive areas. The simulation of this last type of electrode is beyond present-day DFT computational capabilities. Nevertheless, the use of a metallic ideal wire allows one to inspect specifically the defects in a system with a wire-like geometry. Indeed, the strategy of using an ideal wire as an electrode is in common use in the transport study of semiconducting nanowires [36] and carbon nanotubes [37, 38].

Note that the central scattering region includes (i) a finite DB wire with a length between 2 and 5 DBs and (ii) two H-passivated dimers placed at each end of this DB wire (see figure 13). These H-junctions are used to decouple the central DB wire from the leads, as explored above. As a result, one can converge the different solutions corresponding to the different states of the DB wire, while the leads remain as ideal DB wires.

As one can then expect, the effect of two H-passivated dimers is to confine the DB wire states, leading to a particle-in-a-box behavior. If, instead of using the open boundary conditions, one uses periodic conditions, these confined states will appear as essentially flat bands within the bulk gap, as can be seen in figure 14 for the example of a 5 DB ideal wire (blue solid lines). The corresponding transmission
exhibits peaks and dips that can be understood by examining the confined states.

The three first states of an ideal 5 DB wire give clear resonance peaks in the transmission spectrum. They are within the energy range of the one-channel energy range of the ideal DB wire lead, i.e. \(0.53 \text{ eV} < E - E_F < 0.08 \text{ eV}\). On the other hand, the states located in the two-channel energy range result from a mixing between the states of the DB wire and the ones from the leads. As a result, the transmission spectrum does not display resonance peaks but an overall enhancement in the high energy range of the two-channel band.

The \(T(E)\) spectral behavior is similar for an NM wire (see figure 15). In the case of a 5 DB NM wire, the DB wire’s states also give rise to \(T(E)\) resonances. A larger transmission is obtained for a DB wire state coupled with a state of the leads (see figure 16). In the two-channel energy range, the \(T(E)\) spectrum is the one observed in the case of H-junctions (see figure 3). Indeed, as opposed to the 5 DB ideal wire, the transmission is not perturbed by wire’s states that are shifted and give resonance peaks at higher energies. When going from a 2 to a 5 DB NM wire, the overall shape of the transmission spectrum remains the same but with a larger number of resonance peaks corresponding to an increasing number of DBs in the wire (see figure 17).

In the same manner, the transmission through a 5 DB AFM wire exhibits resonances corresponding to states localized within the wire (see figure 18). Nevertheless, these states are confined below \(E - E_F = -0.3 \text{ eV}\) and above \(0.3 \text{ eV}\), leaving the transmission largely undisturbed. The situation is the same whatever the length of the wire (see figure 19). Let us stress that the difference between the transmissions of the majority and minority spins in the case of odd finite length DB wires is due to the monoreferencial nature of the DFT approach, which cannot deliver proper spin states. We observe an exponential decay of the transmission away from the resonances. Thus, one can define and evaluate, as in the H-junction case, an inverse decay length for the AFM wire. The calculated value, \(\gamma_{AFM} = 0.89 \text{ Å}^{-1}\), at \(E - E_F = 0.15 \text{ eV}\).

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4 Let us note that some resonance peaks are pushed outside of the energy range defined by the leads and, thus, do not show up in the \(T(E)\) spectra of figure 17.
Figure 18. The band structure (left) and transmission $T(E)$ (right) of the 5 DB AFM wire. The states localized on the wire are depicted in blue (solid and dashed lines for majority and minority spins, respectively). The states of the electrodes are depicted by black dashed lines. The bands of the electrodes appear to be shifted due to the periodic boundary conditions used to calculate the band structures.

Figure 19. The transmission through AFM wires as a function of energy. (a) 2 DB length, (b) 3 DB, (c) 4 DB and (d) 5 DB. Majority and minority spins are depicted by solid and dashed lines, respectively. The transmission of the ideal wire is depicted in black.

Figure 20. The band structure (left) and transmission $T(E)$ (right) of the 5 DB FM wire. The states localized purely on the wire are depicted in blue (solid and dashed lines for majority and minority spins, respectively). The states of the electrodes are depicted by black dashed lines. The bands depicted by red dotted lines result from a mixing between the electrode and wire states for the minority spin. The bands of the electrodes appear to be shifted due to the periodic boundary conditions used to calculate the band structures.

Figure 21. The transmission through FM wires as a function of energy. The different panels and lines correspond to the same cases as figure 19.

is over three times larger than the one of the H-junctions at the same energy.

The case of the 5 DB FM wire is extremely similar to the previous one (see figure 20). The main difference lies in the energy distribution of the DB wire’s states depending on their spin. Indeed, as expected, the majority spin states occupy a lower range of energy, whereas the minority spin states are found near the two-channel energy range. As a consequence, the transmission spectra are extremely different for the two spins, whatever the length of the finite central DB wire (see figure 21). The energy localization of the resonances is proper for the spin, featuring a spin filter behavior.

This systematic inspection reveals a common feature in the transmission of finite size DB wires due to an overall general behavior of $T(E)$. It is due to the original shape of the ideal DB wire, used here as the electrode. This smooth transmission function is then perturbed by multiple resonances arising from states of the wire confined in between passivated dimers. The positions of these peaks and dips are specific to the nature of the wire, as we have discussed above.
Figures 17, 19 and 21 show the electron transmission coming from an ideal DB wire, transmitting into another ideal DB wire at a given electron energy $E$. As such, it is not easy to deduce the actual electron currents in the studied systems. We computed the electron current using the Landauer–Büttiker formula.

\[
I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E, V) [f_R(E) - f_L(E)] dE,
\]

where $T(E, V)$ is the transmission function for an electron of energy $E$ when the bias between the two DB electrodes is $V$, and $f_R(E)$ ($f_L(E)$) is the right- (left-) electrode Fermi occupation function. We further simplify the calculation of the current $I$ using the zero-bias transmissions of figures 17, 19 and 21. Figure 22 shows the computed $I$–$V$ curves for 5 DB wires in the ideal, NM, AFM and FM configurations. As we can see, the electronic currents of the actual physical wires are very reduced as compared to the current of the ideally undistorted non-magnetic wire.

Our recent study of the total energy and stability of DB wires [16] shows that the AFM and NM solutions are thermodynamically coexisting; however, their very different $I$–$V$ characteristics would permit identification of the type of DB wire obtained.

### 7. Polaronic effects in transport

The above study only considers elastic transport. However, the large electron-vibration coupling leading the DB wires to Jahn–Teller distortions would modify the transport from our above description. Indeed, a DFT-based tight-binding study suggested that transport in infinite DB wires would take place in the form of small-polaron diffusion [9, 39]. Hole polarons are extended over 3 DB sites [9], while electron polarons present a similar confinement [9]. We have estimated the extension of the induced electron polaron by including an extra charge in the NM 5 DB wire. The most noticeable effect is that the distortion changes sign, with DB sites moving away from the surface when before they were moving towards the surface, and vice versa. However, the degree of distortion remains the same. More importantly, the electron is not localized to only three sites, but extends over the full wire, giving rise to no confinement except for the finite size of the DB wire. Hence, the existence of small polarons may be due to the actual extension of the DB wire, implying that transport will take place by polaron hopping only in long wires [39]. Nevertheless, the polaron extension can vary greatly depending on the actual Si system, and atomic extensions are possible [40].

8. Conclusion

In this study, we investigated the electronic transport properties of dangling-bond (DB) silicon wires on H-passivated Si(100). Thanks to DFT calculations and analysis by maximally localized Wannier functions, we have been able to rationalize the transport properties of DB wires subjected to Jahn–Teller distortions and magnetic instabilities and compared with ideal DB wires. This study shows that transport mainly proceeds via subsurface atoms because the through space DB interaction is negligibly small. Only a hydrogen impurity is then efficient in interrupting the subsurface transport because it decouples the subsurface states from the surrounding DBs.

Different finite size dangling-bond wires have been studied. We have considered unperturbed, Jahn–Teller distorted, antiferromagnetic and ferromagnetic wires containing 2, 3, 4 and 5 DBs. Each wire displays typical and unique trends in transmission, allowing us to characterize the nature of the wire from its transport properties. The sizes of the studied wires are of the order of the small-polaron extension of DB wires [9], producing a shifting of the electronic structure but qualitatively similar features. Hence, we expect polaronic effects to be important mainly in long wires.

The results of this work show that instabilities greatly reduce the conductance of the wires as compared with ideal wires, hence making 1-D effects a dominant effect in electron transport in DB wires. Moreover, each type of studied DB wire has a distinctive transmission function leading to starkly

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**Figure 22.** The calculated current (nA) with respect to the bias (V) for 5 DB wires. Ideal, NM, AFM and FM wires are displayed from the top to the bottom.
different $I-V$ characteristics. These are strong fingerprints of the corresponding wires permitting us to use the $I-V$ characteristics as a wire spectroscopy technique which should help in unambiguously determining the type of DB wire experimentally accessible [8].

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