

**Soliton effects in dangling-bond wires on Si(001)**C. F. Bird,\* A. J. Fisher,<sup>†</sup> and D. R. Bowler<sup>‡</sup>*Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom*

(Received 30 January 2003; revised manuscript received 7 May 2003; published 26 September 2003)

Dangling bond wires on Si(001) are prototypical one-dimensional wires, which are expected to show polaronic and solitonic effects. We present electronic structure calculations, using the tight binding model, of solitons in dangling-bond wires, and demonstrate that these defects are stable in even-length wires, although approximately 0.1 eV higher in energy than a perfect wire. We also note that in contrast to conjugated polymer systems, there are two types of soliton and that the type of soliton has strong effects on the energetics of the band gap edges, with the formation of intragap states between 0.1 and 0.2eV from the band edges. These intragap states are localized on the atoms comprising the soliton.

DOI: 10.1103/PhysRevB.68.115318

PACS number(s): 68.65.-k, 73.20.-r, 71.15.Nc, 71.38.+k

**I. INTRODUCTION**

There are many motivations to understand the transport properties of materials in the extreme one-dimensional limit. Some are technological: the logical conclusion to the historic reduction in size of electronic components would be active device elements, and passive connections between them, that are of atomic scale. There has been much recent interest in structures that might act as atomic-scale wires<sup>1</sup> or as atomic- or molecular-scale switches. Other reasons relate to fundamental physics: transport in one dimension is very different to higher dimensions, because the coupling of electrons to other excitations, both of the lattice and of the electronic system, is strong. This can lead to instabilities such as the formation of a Luttinger liquid<sup>2</sup> or one of a Peierls<sup>3</sup> (infinite wire) or Jahn-Teller<sup>4</sup> (finite wire) distortion, with correspondingly strong modifications to transport properties.

One striking example of this type of behavior is in conductive polymer systems.<sup>5</sup> These exhibit an alternation of double and single bonds which is at least partly of the classic Peierls type (driven by electron-lattice coupling), although electron correlation effects may also be important.<sup>6</sup> Carriers introduced into these systems are localized, probably partly by disorder but also to a significant degree by self-trapping by the lattice.<sup>7</sup> There are two main classes of charged defect; one is the polaron, which is similar in principle to excitations in higher-dimensional systems. Here the carrier is surrounded by a region in which the atomic distortions serve to lower its own energy (in this case, involving a reduction in the double-single bond alternation). The second type is the soliton; this can occur only in “degenerate” systems, such as *trans*-polyacetylene (t-PA), where there are two equivalent ground states of an infinitely long chain, in which the double and single bonds are interchanged. The soliton involves a midgap state associated with a “domain wall” between regions of opposite bond alternation. Although localized, both polarons and solitons are highly mobile, and much is known about their effect on transport in both the coherent and incoherent limits.<sup>5,8,9</sup>

In this paper, we examine an alternative pseudo-one-dimensional system based on the “dangling-bond wire.” This system is formed on a hydrogen terminated silicon (001) surface via scanning tunneling microscopy induced selective desorption of hydrogen along the edge of a dimer

row.<sup>10</sup> The atoms in such wires have been shown (both theoretically and experimentally) to undergo a Peierls/Jahn-Teller type distortion, giving rise to an alternating pattern of atomic positions with respect to those of the passivated surface, and producing the electronic structure of a one-dimensional narrow-gap semiconductor.<sup>10</sup> In contrast to the conducting polymers, this distortion occurs predominantly perpendicular to the axis of the “wire”; however, as in the conductive polymers, the resulting structure is not expected to be “static.” We recently predicted,<sup>11</sup> on the basis of tight-binding calculations, that electrons or holes introduced into such wires will produce self-trapped “small polaron” defects. Despite their localization, we have also shown that these defects are remarkably mobile near room temperature and above,<sup>12</sup> raising the interesting possibility of the transport of charge through such devices.

It is natural to ask whether there might be solitonic, as well as polaronic, defects in dangling-bond wires (as in t-PA); after all, these structures are degenerate (the total energy is invariant under exchanging the “up” and “down” atoms). This question is intimately related to the effect of different types of boundary condition; in the case of t-PA, double bonds are “anchored” at the ends of the chain, so that the ground state of a neutral chain with odd length contains a bond-alternation defect (soliton) at the center. The behavior in t-PA is simple because the energy scales for the binding of double bonds to the ends of the chain are much larger than any involved in the formation of defects along it.

In this paper we explicitly focus on the behavior of dangling-bond wires of finite length, with a view to studying the formation of charge-neutral solitons and the end effects. We find that the situation is more complicated than in t-PA, because the energy scales of the end effects and the defects are comparable to one another. This means that there is a much more complex behavior when deliberate defects are introduced into the alternating pattern. Accordingly we pay particular attention to the stability of various possible defects and their contributions to the electronic structure of the wire. In light of the large number of possible initial configurations and the necessarily large system size (>400 atoms), we chose to use a semiempirical tight-binding approach<sup>13</sup> that was fast enough to allow a comprehensive study of possible

defects and had accurate parametrizations available for the system under consideration.

## II. TECHNICAL DETAILS

### A. Basic configuration and relaxation parameters

A silicon slab was constructed out of six layers, parallel to the (001) plane. Each layer had a  $4 \times 12$  array of silicon atoms positioned at the appropriate positions for a perfect “diamond” lattice, with the “bottom” layer terminated with hydrogen atoms. This layer and the associated hydrogen atoms were not allowed to move during relaxation, and represented the bulk. The unterminated upper surface was allowed to reconstruct to form a pair of dimer rows. This (001) surface was then terminated with hydrogen atoms to produce a fully terminated slab that served as a basis for all the simulations. This unit cell contained 432 atoms.

Each slab was separated from its neighbors by a vacuum gap of  $15 \text{ \AA}$  once periodic boundary conditions were applied. For the maximum length considered of eight dangling bonds, each wire was isolated by four hydrogen terminated atoms from its virtual neighbors along the wire direction, while shorter wires had proportionately greater numbers of hydrogen terminated atoms at each end. All wires were isolated by a completely terminated dimer row from adjacent wires once periodic boundaries were considered, as this has been found to provide adequate isolation.<sup>14</sup>

Wires were created by removing the required number of terminating hydrogen atoms from the upper surface, along one side of a dimer row. The reference point for distortions was the average position of hydrogen terminated silicon atoms in the passivated surface, labeled as the baseline or “level” position. Displacements normal to the surface in the direction of the bulk were “down,” and those away from the bulk were “up.” Before relaxation, up atoms were displaced by an additional  $0.3 \text{ \AA}$  compared to terminated atoms of the normal spacing, and down atoms by  $0.4 \text{ \AA}$  less than terminated atoms.

Previous work<sup>15</sup> examined the effect of slightly perturbing the starting positions to determine whether the final results were stable with respect to small distortions, and found that this was the case. Accordingly only one magnitude of starting displacement was considered in this study.

All relaxations and electronic structure calculations were performed using the Oxford Order-N (OXON) tight-binding package.<sup>13</sup> Structural relaxations were performed at a system temperature of 0 K until the maximum force per atom reached the limit of  $0.01 \text{ eV/\AA}$ . The majority of simulations required on the order of 150 iterations to relax. The Hamiltonian was solved using exact diagonalization, and periodic boundary conditions were applied to the simulation. Spin polarization was not included in the calculations. The silicon parametrization used was that of Bowler *et al.*,<sup>16</sup> which was specifically fitted for the Si(001) surface and hydrogen on that surface. It is worth noting that this parametrization did not fit to the conduction band, so that absolute values should not be trusted, though generic behaviors (such as shifts in levels) are likely to be correct.

TABLE I. Total energies (eV) calculated for relaxed perfectly ordered three and eight-atom-long chains at 0 K as a function of  $k$ -point mesh size.

Mesh size	Three-atom chain	Eight-atom chain
$1 \times 1 \times 1$	-1963.7827	-1948.6625
$1 \times 2 \times 1$	-1963.7828	-1948.6625
$2 \times 1 \times 1$	-1964.1376	-1949.0197
$2 \times 2 \times 1$	-1964.1377	-1949.0197
$2 \times 4 \times 1$	-1964.1377	—
$4 \times 1 \times 1$	-1964.1364	-1949.0183
$4 \times 2 \times 1$	-1964.1365	—
$4 \times 4 \times 1$	-1964.1365	—
$4 \times 4 \times 4$	-1964.1365	—

Convergence of the total energy was tested with respect to the  $k$ -point mesh. An initial search was performed with a three atom wire to minimize the calculation time, and selected results replicated with an eight atom wire. Table I shows the results of the convergence calculations. Results were adequately converged ( $0.01 \text{ eV}$ ) using a Monkhorst-Pack<sup>17</sup>  $2 \times 1 \times 1$  grid, and all simulations presented below used such a mesh.

### B. Configurations considered

Dangling-bond (DB) wires four, six, and eight atoms long were considered. Some simulations of odd-length wires were performed, but these were not pursued for reasons discussed below in Sec. III A. Each wire was considered initially with perfect structure, i.e., the initial starting positions were alternately up then down (or vice versa). Defects were then introduced consisting of two adjacent up atoms or two adjacent down atoms at all possible positions in the wire, with the remaining atoms alternating appropriately. All defects were neutral. An example of an eight atom wire with a down-down defect is shown in Fig. 1.

## III. RESULTS

### A. End effects

We have previously tested the use of tight binding for infinite dangling bond wires,<sup>11,12</sup> obtaining a good agreement with experiment and *ab initio* results. However, when we came to examine finite wires with an odd number of sites, we found an anomaly: one site on the wire became “level” (i.e., at the same height as if it were hydrogenated) and the rest of

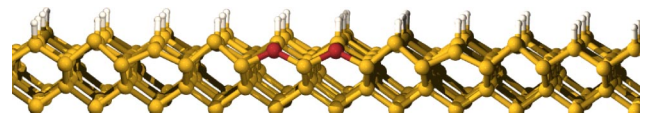


FIG. 1. A DB wire of length eight, with a DD soliton in the middle (marked with darker atoms). The image shows only the top four layers of silicon, and limited terminating hydrogens (one on the left and two on the right).

the wire behaved as a wire with an even number of sites, in contrast to *ab initio* results. The local charge on the level atom was zero, again in contrast to the rest of the wire (where down atoms showed a charge deficit and the up atoms showed a charge excess). In this section, we explore the reasons for this behavior and investigate whether tight binding is a viable technique for such systems.

The shortest, and simplest, finite wires of odd and even length for which there are experimental data are those with three and four sites, respectively<sup>10</sup> (the length 2 wire might be too short, as it effectively consists of only end atoms). We have already performed extensive investigations of this system using spin-polarized density functional theory, and found good agreement with experiment.<sup>18</sup> In particular, we found that the length 3 wire has a rather small displacement pattern (with the two end atoms 0.11 Å higher than the central atom), in close agreement with experiment (where displacements of 0.15 Å are measured), and that the length 4 wire can form alternating up/down or down/up patterns, or an up/down/down/up pattern.

Our tight binding simulations of even length wires were in good agreement both with the experimental results and the density functional theory (DFT) simulations. In order to better understand the peculiar behavior for the odd length wires, we used local charge neutrality (LCN) Ref. 19 (where the on-site energies of individual atoms are adjusted until their net charge is zero) to remove any charge transfer effects in the tight-binding simulations [it is worth noting that it is still perfectly possible to obtain buckled dimers on the clean Si(001) surface with a LCN condition—we consider the effects on an even length wire below]. The length 3 wire became almost flat under this condition—though the two end atoms were 0.06 Å higher than the central atom, in qualitative agreement with experiment and DFT modeling. We also modeled the length 4 wire with LCN, and found little change—the alternating up/down pattern was still observed. However, the LCN simulations were extremely hard to converge, and did not show particularly improved results. We conclude that, for odd length wires, there is spurious charge transfer that makes modeling these systems potentially inaccurate in tight binding, and we will not consider them further.<sup>20</sup> However, for even length wires there is no problem and we will continue to model these using tight binding with confidence.

### B. Solitons in even length wires

Simulations were performed for chain lengths of four, six, and eight dangling-bond systems. Initial configurations were chosen so as to include all possible permutations of single position ordering defects, for both up and down types. All relaxations successfully converged to the force limit. The results are shown in detail in Table II, but in summary both **uu** and **dd** soliton defects could be formed in the relaxed wire. Compared to a perfectly ordered wire, those containing solitons are approximately 0.1 eV less stable. No soliton defects formed on the end atoms, and there was strong periodicity in possible locations of the defects, as seen in the table.

As well as showing the final, relaxed configuration of the wires (with up atoms notated “u,” down atoms “d,” and

TABLE II. Final structure, energy change, valence and conduction band offsets, and starting structure for soliton-containing even-length wires.  $E_{\text{diff}}$  represents difference in total energy relative to a perfect wire. All energy differences are in electron volts. Soliton defects are shown in bold. VB stands for valence band, and CB for conduction band.

Final	$E_{\text{diff}}$	VB offset	CB offset	Initial
udud	—	—	—	udud
dudu	—	—	—	dudu
udud	—	—	—	<b>ddud</b>
udud	—	—	—	<b>uduu</b>
<b>uddu</b>	0.111	-0.003	-0.109	<b>uddu</b>
<b>uddu</b>	0.111	-0.003	-0.110	<b>uudu</b>
<b>duud</b>	0.102	0.224	0.012	<b>duud</b>
<b>duud</b>	0.101	0.224	0.012	<b>dudd</b>
dududu	—	—	—	dududu
ududud	—	—	—	ududud
ududud	—	—	—	<b>ddudud</b>
ududud	—	—	—	udud <b>uu</b>
<b>uddudu</b>	0.114	-0.003	-0.106	<b>uddudu</b>
<b>uddudu</b>	0.114	-0.002	-0.106	<b>uududu</b>
<b>ududdu</b>	0.114	-0.002	-0.106	<b>uduuud</b>
<b>ududdu</b>	0.114	-0.002	-0.106	<b>ududdu</b>
<b>duudud</b>	0.104	0.226	0.007	<b>duddud</b>
<b>duudud</b>	0.104	0.226	0.006	<b>duudud</b>
<b>duduud</b>	0.104	0.226	0.007	<b>dududd</b>
<b>duduud</b>	0.104	0.226	0.007	<b>duduud</b>
dudududu	—	—	—	dudududu
udududud	—	—	—	udududud
dudududu	—	—	—	<b>dudududd</b>
dudududu	—	—	—	<b>uudududu</b>
<b>uddududu</b>	0.115	0.000	-0.102	<b>uddududu</b>
<b>uddududu</b>	0.115	0.000	-0.103	<b>uduududu</b>
<b>ududdudu</b>	0.117	-0.001	-0.105	<b>ududdudu</b>
<b>ududdudu</b>	0.117	0.000	-0.105	<b>uduuudu</b>
<b>udududdu</b>	0.115	0.000	-0.102	<b>udududdu</b>
<b>udududdu</b>	0.115	0.001	-0.102	<b>udududuu</b>
<b>duududud</b>	0.104	0.228	0.003	<b>ddududud</b>
<b>duududud</b>	0.105	0.227	0.004	<b>duududud</b>
<b>duduudud</b>	0.106	0.230	0.009	<b>duddudud</b>
<b>duduudud</b>	0.106	0.230	0.009	<b>duduudud</b>
<b>dududuud</b>	0.104	0.227	0.003	<b>dududdud</b>
<b>dududuud</b>	0.104	0.228	0.003	<b>dududuud</b>

atoms associated with a soliton in bold) and various energies, Table II shows the initial configuration for each system. It is important to note that several different initial configurations led to the same final configuration (for reasons discussed below).

The effects of the ends of the wire are rather small (only a few meV), but seem to exert a small attractive force on the solitons. More interesting is the apparent instability of solitons of both kinds exactly at the ends of the wire (and of certain configurations with the solitons in the middle of the wire). For instance, the third and fourth lines of Table II

TABLE III. Values of the band gap in even-length wires containing various defects. VB stands for valence band, CB for conduction band, all energies are in eV.

Length	Defect	VB Edge	CB Edge	Bandgap
4	Perfect	-7.66	-6.35	1.31
	<b>dd</b>	-7.66	-6.46	1.20
	<b>uu</b>	-7.44	-6.33	1.11
6	Perfect	-7.66	-6.36	1.30
	<b>dd</b>	-7.66	-6.46	1.20
	<b>uu</b>	-7.43	-6.35	1.08
8	Perfect	-7.66	-6.36	1.30
	<b>dd</b>	-7.66	-6.46	1.20
	<b>uu</b>	-7.43	-6.35	1.08

show that the initial configurations DDud and UUdu relaxed back to perfect wires, while the eighth line shows that duDD relaxed back to dUUD. This pattern can be easily understood in terms of charge balance: an up atom is associated with an excess of charge, while a down atom is associated with a deficit of charge. The configurations which were unstable (which includes all systems with a single soliton at the end of the wire) had different numbers of up and down atoms, which would lead to charge imbalance, so they changed to a stable configuration with equal numbers of up and down atoms, either removing the soliton entirely or changing it.

Looking at the electronic structure of relaxed wires containing solitons, the presence of a soliton reduced the band gap. The general pattern is that a DD type defect lowered the bottom of the conduction band, while a UU type defect raised the top of the valence band. The values for different length wires are shown in Table III. If the soliton was of the DD type, the bottom of the conduction band was lowered by 0.1 eV, while the top of the valence band was raised by 0.22 eV by the presence of an UU defect. Both these effects were due to the introduction of an intragap state, as illustrated in Fig. 2. We recall that the system was not parametrized for the conduction band, and accordingly absolute energies relating to it should be treated with caution. We also note that the value of the gap is in good agreement with our previous calculations on the system.<sup>11</sup>

A soliton is generally associated with a midgap state, which is seen here in the change of the valence and conduction bands. These effects can be understood in terms of the hybridization of the silicon making up the surface: in ideal, bulk positions the atoms are  $sp^3$  hybridized, but reconstruction into dimers at the surface pulls the atoms away from this state. When Jahn-Teller distorted, either during buckling of dimers or forming a finite length DB wire as here, the atoms displaced up move closer to  $sp^3$  hybridization and gain charge (tending to a lone pair) while the atoms displaced down move closer to  $sp^2$  hybridization with a lone  $p$  orbital and lose charge (tending to an empty dangling bond). Thus the up atoms are associated with filled states at the top of the valence band, while the down atoms are associated with empty states at the bottom of the conduction band. The up and down displacements affect the underlying substrate (in

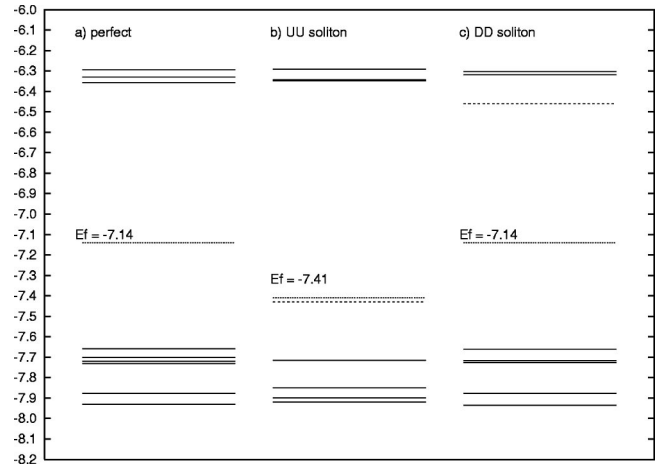


FIG. 2. Energies (eV) of states adjacent to the band gap for (a) perfectly ordered eight atom wire, (b) an eight atom wire with a UU defect, and (c) an eight atom wire containing a DD defect. The Fermi level is shown as  $E_f$ .

particular the second and third layer atoms) in such a way that alternating up and down displacements (either along or across a dimer row) are energetically favorable. When this is interfered with, as in a soliton, the extent of the relaxation towards  $sp^3$  or  $sp^2+p$  is reduced, and the band edges are affected. This is in marked contrast to conjugated polymers, as will be discussed below.

We display the physical displacement of the atoms for a finite, nondistorted wire, and wires with both types of soliton, in Fig. 3. We also show by dotted lines, the heights of atoms in a perfect wire (up and down) and a hydrogenated wire. We can see a number of effects in the figure. First, the end atoms are slightly depressed relative to the perfect wire positions, as we might expect—they are slightly more con-

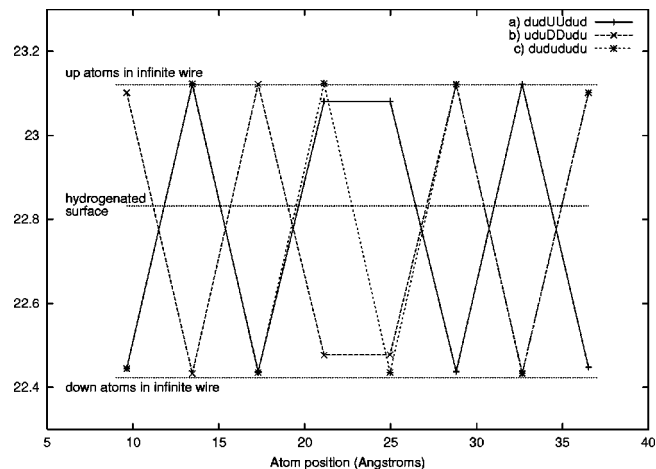


FIG. 3. Effects of soliton formation on the displacement of atoms forming finite DB wires. We plot the absolute vertical position ( $\text{\AA}$ ) of atoms forming the wire in systems containing (a) a central UU soliton, (b) a central DD soliton, and (c) a perfect alternating wire. The positions of equivalent silicon atoms in a perfectly hydrogenated surface and of up and down atoms in an infinite wire are shown by horizontal dotted lines.

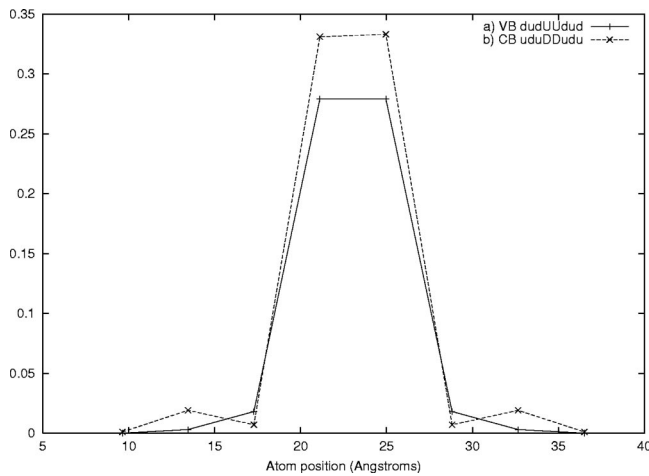


FIG. 4. Effects of soliton formation on the electronic structure of finite DB wires. We plot contributions to the wave function for specific bands from atoms most strongly affected as a function of distance along the wire: (a) Highest occupied electronic state for a central UU soliton, (b) Lowest unoccupied electronic state for a central DD soliton.

strained. Second, the atoms in the solitons are pulled away from the perfect wire positions considerably: the DD soliton atoms are moved up, and the UU soliton atoms moved down. Finally, the neighbors of the solitons are unaffected by the defect: their heights are essentially equivalent to the perfect wire positions.

We can analyze the electronic structure of the solitons by looking at the contributions to the appropriate wave functions from the atoms in the system, as plotted in Fig. 4. We show the contributions to the highest occupied band for a UU defect and to the lowest unoccupied band for a DD defect. These show that the gap states are strongly localized on the defect atoms, and have almost no contributions from neighboring atoms. The overall structures of the defects are similar to that of the polaron seen in the same system,<sup>11,12</sup> and indicates that the soliton is similarly weakly coupled to the bulk. The overall behavior and form of the soliton in the DB wire are very different from the conjugated polymer system. In particular, the soliton is associated with a pair of

atoms and has two forms, while in conjugated polymers it is associated with the bond lengths near a single atom, and has only one form.

#### IV. DISCUSSION AND CONCLUSIONS

Although the dangling-bond system is too reactive to be a component of nanoscale circuitry, it does serve both as a potential model for the study of one-dimensional conductors and as a stepping stone to realizable useful systems, for example as a template for the deposition of metal atoms in linear features. As such it is important that systems can be modeled accurately and quickly. In this paper, we have demonstrated that tight-binding simulations are suitable for even-length wires, and used such techniques to explore the stability of ordering defects in the Jahn-Teller alternating displacement seen in perfect dangling-bond wires. We note that the modeling of odd-length wires is complicated by the development of “level” atoms in the relaxed system. This appears to be related to difficulties in adequately modeling unpaired electrons using the tight-binding formalism; we have modeled these systems using spin-polarized DFT, reported elsewhere.<sup>18</sup>

In the even length system, we demonstrate that soliton-type defects, where alternation between up and down displacements is interrupted, are only  $\sim 0.1$  eV less stable than the perfect wire, but are associated with strong effects on the edges on the valence and conduction bands, as shown in Fig. 2, as a consequence of changes in the hybridization state. The presence of a “UU” defect leads to the formation of an isolated state 0.22 eV above the original valence band. A “DD” defect is associated with a state 0.1 eV below the original conduction band, although the conduction band energies should be treated with caution due to the nature of the parametrization. We also demonstrate that these states contain large contributions from the atoms associated with the defect, i.e., localization.

#### ACKNOWLEDGMENTS

We thank the UK Engineering and Physical Sciences Research Council for funding (C.F.B.) and the Royal Society for a University Research Fellowship (D.R.B.).

\*Electronic address: c.bird@ucl.ac.uk

<sup>†</sup>Also at London Center for Nanotechnology, Gordon St, London WC1E 6BT, United Kingdom.

Electronic address: andrew.fisher@ucl.ac.uk

<sup>‡</sup>Also at London Center for Nanotechnology, Gordon St, London WC1E6BT, United Kingdom.

Electronic address: david.bowler@ucl.ac.uk

<sup>1</sup>J. Lyding, T.-C. Shen, J. Hubacek, J. Tucker, and G. Abeln, Appl. Phys. Lett. **64**, 2010 (1994).

<sup>2</sup>F. Haldane, J. Phys. C **14**, 2585 (1981).

<sup>3</sup>R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, Oxford, 2001), p. 108 ff., Oxford Classics Series, reprint of 1936 original.

<sup>4</sup>H. A. Jahn and E. Teller, Proc. R. Soc. London, Ser. A **161**, 220 (1937).

<sup>5</sup>A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W. P. Su, Rev. Mod. Phys. **60**, 781 (1988).

<sup>6</sup>G. König and G. Stollhoff, Phys. Rev. Lett. **65**, 1239 (1990).

<sup>7</sup>L. Landau, Phys. Z. Sowjetunion **3**, 664 (1933).

<sup>8</sup>H. Ness and A. Fisher, Phys. Rev. Lett. **83**, 452 (1999).

<sup>9</sup>H. Ness and A. Fisher, Europhys. Lett. **57**, 885 (2002).

<sup>10</sup>T. Hitosugi, S. Heike, T. Onogi, T. Hashizume, S. Watanabe, Z. Q. Li, K. Ohno, Y. Kawazoe, T. Hasegawa, and K. Kitazawa, Phys. Rev. Lett. **82**, 4034 (1999).

<sup>11</sup>D. R. Bowler and A. J. Fisher, Phys. Rev. B **63**, 035310 (2001).

<sup>12</sup>M. Todorovic, A. Fisher, and D. Bowler, J. Phys.: Condens. Matter **14**, L749 (2002).

<sup>13</sup>C. M. Goringe, D. R. Bowler, and E. Hernandez, Rep. Prog. Phys. **60**, 1447 (1997).

<sup>14</sup>S. B. Healy, C. Filippi, P. Kratzer, E. Penev, and M. Scheffler,

- Phys. Rev. Lett. **87**, 016105 (2001).
- <sup>15</sup>C. F. Bird, MSci Project Report, CMMP, Physics Dept., University College London (2001); URL [http://www.cmmp.ucl.ac.uk/~cfb/DB\\_wire\\_Si.pdf](http://www.cmmp.ucl.ac.uk/~cfb/DB_wire_Si.pdf).
- <sup>16</sup>D. R. Bowler, M. Fearn, C. M. Goringe, A. P. Horsfield, and D. G. Pettifor, J. Phys.: Condens. Matter **10**, 3719 (1998).
- <sup>17</sup>H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).
- <sup>18</sup>C. F. Bird and D. R. Bowler, Surf. Sci. **531**, L351 (2003).
- <sup>19</sup>A. P. Sutton, M. W. Finnis, D. G. Pettifor, and Y. Ohta, J. Phys. C **21**, 35 (1988).
- <sup>20</sup>If two length 3 wires are modeled on adjacent dimer rows, one shows an up/down/up pattern and the other a down/up/down pattern, showing that, while tight binding allows charge transfer too easily, it can model the basic physics of the system correctly.