

## First-principles study on electron transport of carbon dumbbells C60-Cn-C60

R. N. Wang, X. H. Zheng, L. L. Song, and Z. Zeng

Citation: *J. Chem. Phys.* **135**, 044703 (2011); doi: 10.1063/1.3613647

View online: <http://dx.doi.org/10.1063/1.3613647>

View Table of Contents: <http://jcp.aip.org/resource/1/JCPSA6/v135/i4>

Published by the [American Institute of Physics](#).

---

### Additional information on *J. Chem. Phys.*

Journal Homepage: <http://jcp.aip.org/>

Journal Information: [http://jcp.aip.org/about/about\\_the\\_journal](http://jcp.aip.org/about/about_the_journal)

Top downloads: [http://jcp.aip.org/features/most\\_downloaded](http://jcp.aip.org/features/most_downloaded)

Information for Authors: <http://jcp.aip.org/authors>

## ADVERTISEMENT



**AIP Advances**

Special Topic Section:  
**PHYSICS OF CANCER**

Why cancer? Why physics? [View Articles Now](#)

# First-principles study on electron transport of carbon dumbbells $C_{60}$ - $C_n$ - $C_{60}$

R. N. Wang,<sup>1,2</sup> X. H. Zheng,<sup>1</sup> L. L. Song,<sup>1,2,3</sup> and Z. Zeng<sup>1,a)</sup>

<sup>1</sup>Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China

<sup>2</sup>Graduate School of the Chinese Academy of Sciences, 19A Yu Quan Rd, Beijing 100049, China

<sup>3</sup>School of Electronic Science and Applied Physics, Hefei University of Technology, Hefei 230009, China

(Received 11 May 2011; accepted 27 June 2011; published online 25 July 2011)

Electronic transport properties of carbon dumbbells, a new type of carbon hybrid nanostructures formed by connecting carbon atomic chains to two fullerenes  $C_{60}$ , are investigated by using nonequilibrium Green's functions in combination with the density-functional theory. Specifically, the transport properties as a function of the carbon chain length  $n$  are examined. An obvious metal-insulator-like oscillation has been achieved with the increase of the carbon chain length. When  $n$  is even, the device behaves as a metal. In contrast, when  $n$  is odd, it behaves as an insulator. It is quite different to the carbon chains directly sandwiched between metallic leads where the low conductance states are observed for even  $n$  while the high conductance states are observed for odd  $n$ . Such a difference arises from the screening effect of  $C_{60}$ s. © 2011 American Institute of Physics. [doi:10.1063/1.3613647]

## I. INTRODUCTION

The continuing miniaturization of electronic devices motivates the search for new low-dimensional semiconductive or conductive materials which strongly differ in their electrical properties from three-dimensional periodic materials and can be used as either nanocontacts or nanoconductors. Particularly, a few prototype carbon nanostructures, such as zero-dimensional fullerene ( $C_{60}$ ),<sup>1–6</sup> one-dimensional carbon atomic wire,<sup>7–18</sup> carbon nanotube (CNT) or graphene nanoribbon (GNR),<sup>19</sup> and two-dimensional graphene have been widely investigated because of their novel electronic properties and promising potentials as building blocks for future electronic devices. Furthermore, in order to extend the functionality of carbon nanostructures, the construction of hybrid structures with CNT,  $C_{60}$ , graphene, and even carbon atomic chain have attracted intense interests recently. For example, nanopeapod<sup>20–23</sup> with  $C_{60}$  encapsulated in CNT, nanobud<sup>24–26</sup> with  $C_{60}$  attached at the sidewall of CNT, and GNR/CNT junction<sup>27</sup> as partially unzipped CNT, have all been fabricated or suggested. One of the interesting features about such hybrid structures is that they have the characteristics of all the individual components. By combining the functions of these components, new properties can even be obtained. Thus, more degree of freedom for function tuning can often be achieved in the devices constructed from these low-dimensional structures.

Recently, a new kind of carbon hybrid nanostructure which is built by connecting a carbon atomic chain to two  $C_{60}$ s has attracted the attention from the researchers. Since the hybrid structure looks like a dumbbell, we call it a “carbon dumbbell” and denote it as  $C_{60}$ - $C_n$ - $C_{60}$  where  $n$  is the number of carbon atoms in the atomic chain. Börrnert *et al.*<sup>28</sup> have performed Born-Oppenheimer molecular-dynamics simulations to study the stability of the  $C_{60}$ - $C_8$ - $C_{60}$  dumbbell and

found that the dumbbell is always stable up to a temperature of 1000 K before the carbon atomic chain disconnects from the  $C_{60}$ s irreversibly. In addition, Liu *et al.*<sup>29</sup> proposed that the carbon dumbbell can be used as an ideal material for hydrogen storage with a hydrogen uptake as high as  $\sim 10$  wt. %. Naturally, for such a new carbon nanostructure, its other physical properties are also worthy of in-depth study. Particularly, in this work, it is our attention to investigate its transport properties by first principles calculations and see how the electron transport properties depend on the individual carbon atomic chain and  $C_{60}$ s.

In fact, as the smallest or thinnest carbon nanostructure, carbon atomic chains have initiated a large number of studies.<sup>8–10</sup> Many interesting electron transport properties have been observed in a device with a carbon atomic chain in direct contact with metallic leads, such as spin-valve effect<sup>12</sup> and negative differential resistance (NDR) (Ref. 13), and the most well-known property is the even-odd oscillatory conductance behavior.<sup>14–18,30,31</sup> Moreover, the electron transport property of  $C_{60}$  has also been widely investigated<sup>4,32–35</sup> and it is shown to be a good conductor when it is sandwiched between two metallic leads due to the charge transfer from the leads to the molecule. Especially, when two  $C_{60}$ s are involved in the devices, NDR is obviously observed as a result of a tunneling mechanism.<sup>5,36</sup> If the two  $C_{60}$ s are doped differently, a good rectification can even be obtained.<sup>37</sup> Furthermore, in several recent molecular junction experiments, the effects of  $C_{60}$ s as anchoring groups connecting the molecules to the electrodes have also been reported.<sup>38,39</sup>

In contrast, in the carbon dumbbell devices which involve both a carbon chain and two  $C_{60}$ s, NDR exists and originates from the alignment of the energy levels of  $C_{60}$ s under finite bias voltages, just like in other devices constructed with two  $C_{60}$ s. In the meantime, the current as a function of bias behaves quite differently for odd  $n$  and even  $n$ . When the carbon chain length  $n$  is even, the current increases rapidly with the bias while for odd  $n$ , it increases very slowly. In order to see

<sup>a)</sup>Electronic mail: zzeng@theory.issp.ac.cn.

the origin of such a big difference, the transport properties of the devices in the equilibrium state with varying chain length  $n$  are systematically examined. With the increase of carbon chain length  $n$ , the even-odd oscillation in the equilibrium conductances is observed, just like in the case with carbon chains directly sandwiched between two metallic leads. However, the low conductance states appear in the cases with odd  $n$  chains while the high conductance states appear for even  $n$  cases. This is exactly opposite to the case with carbon chains directly sandwiched between two metallic leads. Moreover, the low conductance in the odd  $n$  chains is almost as small as zero, which is never observed in the latter cases. Thus an obvious metal-insulator-like oscillation is obtained by increasing the chain length  $n$ . Such a difference is determined to arise from the screening effects of  $C_{60}$ s.

The paper is organized as follows. In Sec. II, we briefly describe the simulation model and computational details. The results and discussions are presented in Sec. III. The paper ends with Sec. IV where a short summary is given.

## II. SIMULATION MODEL AND CALCULATION METHOD

In this work, the simulation model adopted is as a  $C_{60}$ - $C_n$ - $C_{60}$  dumbbell being sandwiched between two atomic scale Al (100) contacts with a finite cross section (see Fig. 1). We choose a supercell with a large enough vacuum layer around the electrode in the  $x$  and  $y$  directions so that the device has no interaction with its mirror images. The carbon atomic chains are symmetrically anchored at the hollow site of the hexagons of two  $C_{60}$ s. As a first step, we assume that the carbon atomic chains between the two  $C_{60}$ s are in the ideal cumulene configuration and the initial distance between two C atoms in the chain is set to 1.283 Å which is the C-C bond length of an infinite carbon chain.<sup>8</sup> Then, the whole system is partially relaxed with the SIESTA code<sup>40</sup> until the force acting on each carbon atom is less than 0.04 eV/Å while the electrode Al atoms are kept fixed. The following electrical transport calculations are carried out by using the SMEAGOL program<sup>41</sup> which combines density functional theory with the non-equilibrium Green's function technique.<sup>42</sup> All calculations are performed within the generalized gradient approximation parameterized by Perdew, Burke, and Ernzerhof.<sup>43</sup> The valence electron wave functions are expanded by localized numerical atomic orbitals with the double zeta plus polarized for all elements and the core electrons are modeled by standard nonlocal norm-conserving pseudopotentials.<sup>44</sup>

## III. RESULTS AND DISCUSSIONS

First, taking  $C_{60}$ - $C_7$ - $C_{60}$  and  $C_{60}$ - $C_8$ - $C_{60}$  dumbbells as two examples, the current as a function of the bias is shown in Fig. 2. Within a bias range of 1.0 V, the electronic current of  $C_{60}$ - $C_7$ - $C_{60}$  exhibits remarkably different behaviors from that of  $C_{60}$ - $C_8$ - $C_{60}$ . The current of the dumbbell with a  $C_7$  chain increases linearly and very slowly between 0 V and 0.6 V and this dumbbell shows semiconductive characteristics, while the dumbbell with a  $C_8$  chain displays good metallic  $I - V$  characteristics and the current increases rapidly with the increasing bias voltage. Meanwhile, in both  $C_{60}$ - $C_7$ - $C_{60}$  and  $C_{60}$ - $C_8$ -

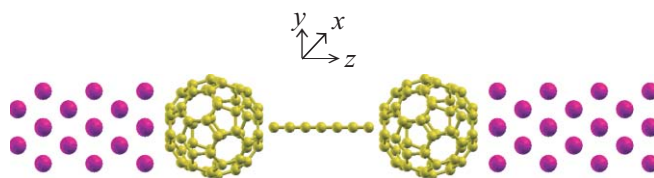


FIG. 1. Schematic illustration of a  $C_{60}$ - $C_n$ - $C_{60}$  dumbbell coupled to Al electrodes which extend to  $z = \pm\infty$ .

$C_{60}$ , NDR is obviously observed around 0.55–0.65 V, where the current decreases with the increasing bias voltage. NDR is essential for certain electronic applications including Esaki diode<sup>45</sup> and most notably resonant tunneling diodes.<sup>46</sup> This behavior has been also reported in other devices involving two  $C_{60}$  molecules and it originates from the tunneling transmission mechanism and the relative shift of the energy levels under the bias.<sup>5,36</sup>

Now we focus on the big difference in the magnitude of the current of  $C_{60}$ - $C_7$ - $C_{60}$  and  $C_{60}$ - $C_8$ - $C_{60}$ . Since the current is determined by the transmission function, it is important to look into the transmission spectra of these dumbbells at zero bias given in Fig. 3. For  $n = 7$ , the transmission in a very big energy range around the Fermi level ( $E_f$ ) is suppressed or completely blocked and thus  $C_{60}$ - $C_7$ - $C_{60}$  is semiconducting. However, for  $n = 8$ , a high transmission peak exists around  $E_f$  which shows that  $C_{60}$ - $C_8$ - $C_{60}$  dumbbell is a good conductor. In order to understand the difference between  $C_{60}$ - $C_7$ - $C_{60}$  and  $C_{60}$ - $C_8$ - $C_{60}$  dumbbells, the projected density of states (PDOS) of C atoms in the carbon chain is shown in Fig. 4, where we only present the PDOS of the first four C atoms of the carbon chains due to the symmetry of the dumbbell structure. In comparison of the transmission in Fig. 3 and the PDOS in Fig. 4, we see that the central C atom plays a dominant role. For  $C_{60}$ - $C_7$ - $C_{60}$ , around  $E_f$ , the density of states decays rapidly from the two sides to the center and the contribution of the central atom is nearly zero. Thus, an effective potential barrier is formed and the electron transmission is blocked (see Fig. 3(a)). On the contrary, in the  $C_{60}$ - $C_8$ - $C_{60}$  system, there is always a peak in the PDOS of all the C atoms in the chain and thus a high transmission peak is observed around  $E_f$  (see Fig. 3(b)).

In fact, the good or poor conductance of the atomic chains was reported to be closely related to the geometry structure of the atomic chain.<sup>47,48</sup> In this work, the bond lengths of

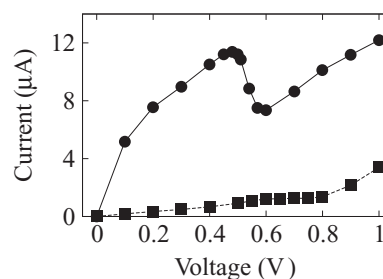


FIG. 2. The current-voltage characteristics of the  $C_{60}$ - $C_7$ - $C_{60}$  (filled square) and  $C_{60}$ - $C_8$ - $C_{60}$  (filled circle) dumbbells, respectively.

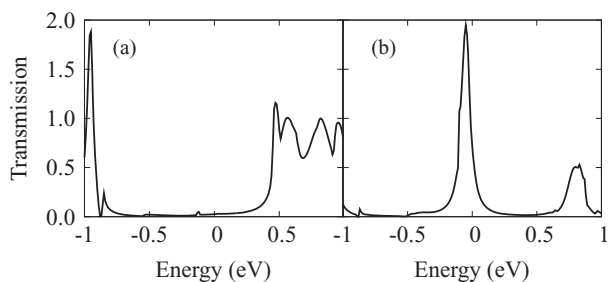


FIG. 3. The transmission spectra of  $C_{60}-C_n-C_{60}$  dumbbells for: (a)  $n = 7$ ; (b)  $n = 8$ . All energy is relative to  $E_f$ .

the odd chains and the even chains are quite different (see Fig. 5). The odd chains are composed by double bonds in a length around 1.23 Å between the adjacent C atoms, while the even chains show alternating single bonds in a length of 1.24 Å and triple bonds in a length of 1.21 Å. Such a difference in bond length arises from the symmetry of the dumbbell. For odd  $n$ , there must be a mirror symmetric plane through a center atom. In this case this atom must make double bonds to its neighbors and all the other bonds thus have to be double bonds. However, if  $n$  is even, the mirror symmetric plane is through a bond. This makes no restriction on the character of that central bond and it could in principle have single, double or triple characters. Due to a Peierls-type distortion, the single and triple bond alternation has much lower energy. In spite of the different bonding styles of carbon atoms in the carbon chain, there are no big differences in relaxed binding geometry between carbon chains and  $C_{60}$  for even  $n$  and odd  $n$ . The lengths between the terminal C to  $C_{60}$  for even and odd systems are 1.33 Å and 1.35 Å, respectively.

Further, the dumbbells with the number  $n$  of the carbon atoms in the atomic chains changing from 3 to 11 are analyzed. Figure 6 shows the equilibrium conductance as a function of  $n$ . The equilibrium conductances are strongly dependent on the number of C atoms in the atomic chain. An

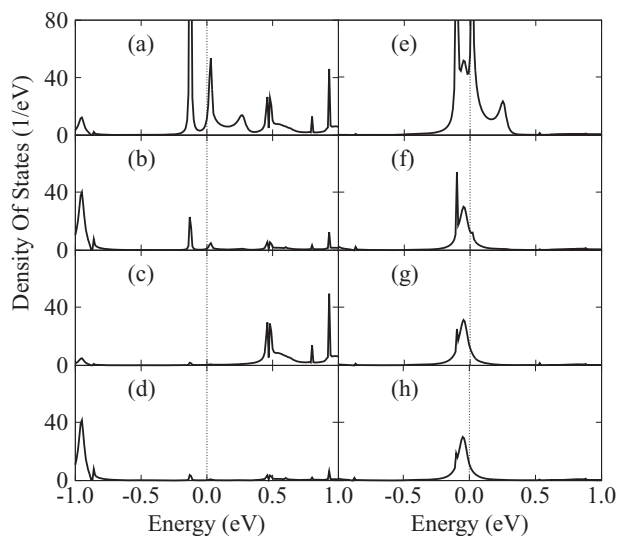


FIG. 4. The PDOS for C atoms of the anchoring carbon atomic chain of  $C_{60}-C_n-C_{60}$  dumbbells: (a)-(d)  $n = 7$ ; (e)-(h)  $n = 8$ . (a)-(d) and (e)-(h) mean the C atoms from the terminal to the center. All energy is relative to  $E_f$ .

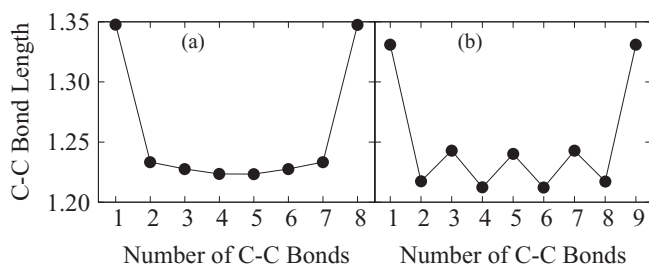


FIG. 5. The C-C bond lengths (in unit of Å) for: (a)  $C_{60}-C_7-C_{60}$ ; (b)  $C_{60}-C_8-C_{60}$ . The first and last bond lengths are those between the terminal carbon atoms in the chain and  $C_{60}$ s.

obvious odd-even oscillation is observed. Very interestingly, for odd  $n$  (except for  $n = 3$ ), the conductance is almost as small as zero ( $\sim 10^{-2} G_0$ ) while for even  $n$ , the conductance is finite ( $\sim 1.0 G_0$ ) and almost constant. In comparison, it is quite different from the case of that the carbon atomic chains are directly sandwiched between two metallic leads where the lower conductance is always around  $1.0 G_0$ .<sup>14,15</sup> Another prominent difference is that, in the dumbbell system, the low conductance states appear in the cases with odd  $n$  chains, while the high conductance states appear for even  $n$  cases. This is exactly opposite to the case with carbon chains directly sandwiched between two metallic leads where low conductance is obtained for even  $n$  and high conductance is observed for odd  $n$ .<sup>14,15</sup> In what follows, we will see how this difference happens.

As is well known, carbon allotropes are usually based on one of the three types of bonding in carbon:  $sp^3$  (diamond),  $sp^2$  ( $C_{60}$ , CNT, GNR, and graphite), and  $sp$  bonding (carbon chain). For carbon chains, the  $2s$  orbital hybridizes with the  $p_z$  orbital to form two  $sp$  orbitals, which covalently bind the adjacent atoms with two  $\sigma$  bonds making the carbon chain linear and stability. Then, the remaining  $p_x$  and  $p_y$  orbitals form  $\pi$  bands, which are 2-fold degenerate and relative to each other by a  $90^\circ$  rotation around the axis. Generally,  $\sigma$  states are localized in the middle of C-C bonds, while  $\pi$  states are centered around single C atoms and delocalized which behave as a one-dimensional free-electron system and are only involved in the conduction process.<sup>49</sup> Each free carbon chain has two pairs of electrons which are not involved in bonding and are largely localized at the end carbon atoms. Thus, for the free  $C_3$  chain the  $\pi$  configuration is  $1\pi(4)$ . When the length of the carbon chain is increased by one carbon atom, two electrons are added to the  $\pi$  orbitals. Therefore, for  $C_4$  chain the  $\pi$  con-

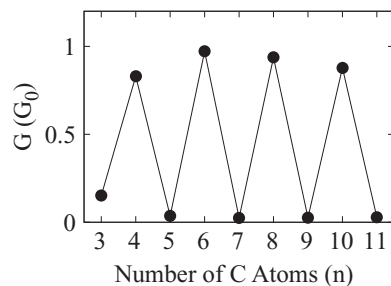


FIG. 6. The equilibrium conductance as a function of chain length  $n$ .



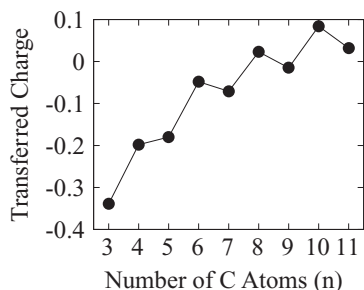


FIG. 7. The extra charge (in unit of  $e$ ) on the atomic chain as a function of the chain length  $n$ .

figuration is  $1\pi(4)2\pi(2)$ . In conclusion, a free  $n$ -atom carbon wire has  $(n-1)/2$  fully occupied  $\pi$  orbitals when  $n$  is odd, and  $(n/2)-1$  fully occupied  $\pi$  orbitals and one half-filled orbital when  $n$  is even.<sup>14,15</sup> It is well known that half-filled orbitals contribute to the electrical conduction while fully occupied orbitals do not. Obviously, this feature will be reflected in the conductance of the carbon chains.

When the carbon atomic wires are directly sandwiched between two metallic leads, there will be a charge transfer process ( $\sim 1.0 e$ ) from the leads to the atomic wire. This  $\sim 1.0 e$  extra charge turns the even  $n$  chain from half filled to fully filled and the odd  $n$  chain from fully filled to half filled. That is the reason why Lang *et al.* got a higher conductance for the odd  $n$  chain and lower conductance for the even  $n$  chain. The charge transfer doping (CTD) plays a key role in turning the chains between half filled and fully filled. However, in the dumbbell structure, we see that the extra charge in the atomic chain is close to 0.0 (see Fig. 7), and very small charge transfer is from the carbon chain to the  $C_{60}$ . Therefore, half filling or full filling is not changed by CTD, which leads to the results that a higher conductance is obtained for even  $n$  chain while a nearly zero conductance is observed for the odd  $n$  chain. The CTD effect is thus negligible here. In fact, the charge transfer from the leads is all collected by the  $C_{60}$ s. Obviously, such a big difference in the dumbbell structures arises from the screening effect of  $C_{60}$ s which block the charge transfer from the metallic leads to the atomic chain. Of course, for  $n = 3$  or 4, we notice that there is a larger charge transfer and it is from the carbon atomic chain to  $C_{60}$ . The carbon atomic chain loses a small amount of charges and the  $\pi$  orbital deviates a little from being fully filled or half filled. This is reflected in the conductance. We see in Fig. 5 that the conductance is a little larger than zero ( $n = 3$ ) or a little decreased ( $n = 4$ ) from other  $n$  even cases.

#### IV. SUMMARY

The electron transport properties of carbon  $C_{60}$ - $C_n$ - $C_{60}$  dumbbell are investigated as a function of the atomic chain length  $n$  by first principles calculations. It is found that such devices show the characteristics contributed both from the  $C_{60}$ s and from the atomic chain. On one hand, NDR is observed, which arises from the electron tunneling between the two  $C_{60}$ s. On the other hand, oscillative conductance is observed with the increase of the carbon chain length. Contrary

to the case with carbon atomic chain directly sandwiched between the metallic leads, low conductance appears in odd  $n$  chains and high conductance appears in even  $n$  chain in the dumbbell system. A remarkable point is that, when  $n$  is odd, the conductance is nearly zero, thus a metal-insulatorlike oscillation is observed with the increase of the carbon chain length. All these interesting behaviors are attributed to the screening effect from the  $C_{60}$ s.

#### ACKNOWLEDGMENTS

This work was supported by the National Science Foundation of China (Grant Nos. 10774148 and 10904148), the special Funds for Major State Basic Research Project of China (973) (Grant No. 2007CB925004), 863 Project, Knowledge Innovation Program of Chinese Academy of Sciences, Director Grants of CASHIPS, and the Scientific Research Foundation for the Returned Overseas Chinese Scholars, State Education Ministry. The calculations were performed at the Center for Computational Science of CASHIPS.

- <sup>1</sup>M. S. Dresselhaus, G. Dresselhaus, and P. C. Eklund, *Science of Fullerenes and Carbon Nanotubes* (Academic, New York, 1996).
- <sup>2</sup>C.-C. Kaun and T. Seideman, *Phys. Rev. Lett.* **94**, 226801 (2005).
- <sup>3</sup>R. Gutierrez, G. Fagas, G. Cuniberti, F. Grossmann, R. Schmidt, and K. Richter, *Phys. Rev. B* **65**, 113410 (2002).
- <sup>4</sup>J. Taylor, H. Guo, and J. Wang, *Phys. Rev. B* **63**, r121104 (2001).
- <sup>5</sup>C. Zeng, H. Wang, B. Wang, J. Yang, and J. G. Hou, *Appl. Phys. Lett.* **77**, 3595 (2000).
- <sup>6</sup>X.-J. Zhang, M.-Q. Long, K.-Q. Chen, Z. Shuai, Q. Wang, B. S. Zou, and Y. Zhang, *Appl. Phys. Lett.* **94**, 073503 (2009).
- <sup>7</sup>C. Jin, H. Lan, L. Peng, K. Suenaga, and S. Iijima, *Phys. Rev. Lett.* **102**, 205501 (2009).
- <sup>8</sup>M. Brandbyge, J.-L. Mozos, P. Ordejon, J. Taylor, and K. Stokbro, *Phys. Rev. B* **65**, 165401 (2002).
- <sup>9</sup>B. Song, S. Sanvito, and H. Fang, *New J. Phys.* **12**, 103017 (2010).
- <sup>10</sup>E. Durgun, R. T. Senger, H. Mehrz, H. Sevincli, and S. Ciraci, *J. Chem. Phys.* **125**, 121102 (2006).
- <sup>11</sup>R. Rivelino, R. B. dos Santos, F. de Brito Mota, and G. K. Gueorguiev, *J. Phys. Chem. C* **114**, 16367 (2010).
- <sup>12</sup>Y. Wei, Y. Xu, J. Wang, and H. Guo, *Phys. Rev. B* **70**, 193406 (2004).
- <sup>13</sup>B. Larade, J. Taylor, H. Mehrz, and H. Guo, *Phys. Rev. B* **64**, 075420 (2001).
- <sup>14</sup>N. D. Lang and P. Avouris, *Phys. Rev. Lett.* **81**, 3515 (1998).
- <sup>15</sup>N. D. Lang and P. Avouris, *Phys. Rev. Lett.* **84**, 358 (2000).
- <sup>16</sup>E. G. Emberly and G. Kirczenow, *Phys. Rev. B* **60**, 6028 (1999).
- <sup>17</sup>B. Wang, Y. Yu, L. Zhang, Y. Wei, and J. Wang, *Phys. Rev. B* **79**, 155117 (2009).
- <sup>18</sup>K. Walczak and G. Platero, *Cent. Eur. J. Phys.* **4**, 30 (2006).
- <sup>19</sup>L. Pisani, J. A. Chan, B. Montanari, and N. M. Harrison, *Phys. Rev. B* **75**, 064418 (2007).
- <sup>20</sup>K. S. Novoselov, Z. Jiang, Y. Zhang, S. V. Morozov, H. L. Stormer, U. Zeitler, J. C. Maan, G. S. Boebinger, P. Kim, and A. K. Geim, *Science* **315**, 1379 (2007).
- <sup>21</sup>J. Lee, H. Kim, S. J. Kahang, G. Kim, Y. W. Son, J. Ihm, H. Kato, Z. W. Wang, T. Okazaku, T. Shinohara, and Y. Kuk, *Nature (London)* **415**, 1005 (2002).
- <sup>22</sup>S. Okada, S. Saito, and A. Oshiyama, *Phys. Rev. Lett.* **86**, 3835 (2001).
- <sup>23</sup>A. Rochefort, *Phys. Rev. B* **67**, 115401 (2003).
- <sup>24</sup>A. G. Nasibulin, P. V. Pikhitsa, H. Jiang, D. P. Brown, A. V. Krashennnikov, A. S. Anisimov, P. Queipo, A. Moisala, D. Gonzalez, G. Lientschnig, A. Hassaniien, S. D. Shandakov, G. Loll, D. E. Resasco, M. Choi, D. Tomanek, and E. I. Kauppinen, *Nat. Nanotechnol.* **2**, 156 (2007).
- <sup>25</sup>J. A. Furst, J. Hashemi, T. Markussen, M. Brandbyge, A. P. Jauho, and R. M. Nieminen, *Phys. Rev. B* **80**, 035427 (2009).
- <sup>26</sup>X. Wu and X. C. Zeng, *Nano Lett.* **9**, 250 (2009).

- <sup>27</sup>H. Santos, L. Chico, and L. Brey, *Phys. Rev. Lett.* **103**, 086801 (2009).
- <sup>28</sup>F. Börrnert, C. Börrnert, S. Gorantla, X. Liu, A. Bachmatiuk, J.-O. Joswing, F. R. Wagner, F. Schaffel, J. H. Warner, R. Schonfelder, B. Rellinghaus, T. Gemming, J. Thomas, M. Knupfer, B. Buchner, and M. H. Rummeli *Phys. Rev. B* **81**, 085439 (2010).
- <sup>29</sup>C. S. Liu, H. An, L. J. Guo, Z. Zeng, and X. Ju, *J. Chem. Phys.* **134**, 024522 (2011).
- <sup>30</sup>J. Prasongkit, A. Grigoriev, G. Wendin, and R. Ahuja, *Phys. Rev. B* **81**, 115404 (2010).
- <sup>31</sup>Y.-H. Zhou, X.-H. Zheng, Y. Xu, and Z. Y. Zeng, *J. Phys.: Condens. Matter* **20**, 045225 (2008).
- <sup>32</sup>C. Joachim and J. K. Gimzewski, *Chem. Phys. Lett.* **265**, 353 (1997).
- <sup>33</sup>J. J. Palacios, A. J. Perez-Jimenez, E. Louis, and J. A. Verges, *Phys. Rev. B* **64**, 115411 (2001).
- <sup>34</sup>T. Ono and K. Hirose, *Phys. Rev. Lett.* **98**, 026804 (2007).
- <sup>35</sup>X. Zheng, Z. Dai, and Z. Zeng, *J. Phys.: Condens. Matter* **21**, 145502 (2009).
- <sup>36</sup>X. H. Zheng, W. Lu, T. A. Abtew, V. Meunier, and J. Bernholc, *ACS Nano* **4**, 7205 (2010).
- <sup>37</sup>X. H. Zheng, X. L. Wang, Z. X. Dai, and Z. Zeng, *J. Chem. Phys.* **134**, 044708 (2011).
- <sup>38</sup>C. A. Martin, D. Ding, J. K. Sorensen, T. Bjornholm, J. M. van Ruitenbeek, and H. S. J. van der Zant, *J. Am. Chem. Soc.* **130**, 13198 (2008).
- <sup>39</sup>E. Leary, M. T. González, C. van der Pol, M. R. Bryce, S. Filippone, N. Martín, G. Rubio-Bollinger, and N. Agrait, *Nano Lett.* **11**, 2236 (2011).
- <sup>40</sup>J. M. Soler, E. Artacho, J. Gale, D. A. Garcia, J. Junquera, P. Ordejon, and D. Sanchez-Portal, *J. Phys.: Condens. Matter* **14**, 2745 (2002).
- <sup>41</sup>A. R. Rocha, V. M. Garcia-Suarez, S. Bailey, C. Lamber, J. Ferrer, and S. Sanvito, *Phys. Rev. B* **73**, 085414 (2006).
- <sup>42</sup>A.-P. Jauho, N. S. Wingreen, and Y. Meir, *Phys. Rev. B* **50**, 5528 (1994).
- <sup>43</sup>J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
- <sup>44</sup>D. R. Hamann, M. Schluter, and C. Chiang, *Phys. Rev. Lett.* **43**, 1494 (1979).
- <sup>45</sup>S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed. (Wiley, New York, 1981).
- <sup>46</sup>R. H. Mathews, J. P. Sage, T. C. L. G. Sollner, S. D. Calawa, C.-L. Chen, L. J. Mahoney, P. A. Maki, and K. M. Molvar, *Proc. IEEE* **87**, 596 (1999).
- <sup>47</sup>A. Calzolari, N. Marzari, I. Souza, and M. B. Nardelli, *Phys. Rev. B* **69**, 035108 (2004).
- <sup>48</sup>Z. Zanolli, G. Onida, and J.-C. Charlier, *ACS Nano* **4**, 5174 (2010).
- <sup>49</sup>S. Cahangirov, M. Topsakal, and S. Ciraci, *Phys. Rev. B* **82**, 195444 (2010).