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The order of references [41]–[52] on page 9 of the published article is shown incorrectly. The authors are very sorry for the mistake and any inconvenience caused. The corrected references are shown below:

[41] Wolf S A, Awschalom D D, Buhrman R A, Daughton J M, von Molnar S, Roukes M L, Chtchelkanova A Y and Treger D M 2001 Science 294 1488
[42] Zutic I, Fabian J and Das Sarma S 2004 Rev. Mod. Phys. 76 323
[43] Makarova T L, Sundqvist B, Hohne R, Esquinazi P, Kopelevich Y, Scharff P, Davydov V A, Kashevarova L S and Rakhmanina A V 2001 Nature 413 716
[44] Hohne R and Esquinazi P 2002 Adv. Mater. 14 753
[45] Sahoo S, Kontos T, Furer J, Hoffmann C, Graber M, Cottet A and Schonenberger C 2005 Nature Phys. 1 99
[46] Tombros N, van der Molen S J and van Wees B J 2006 Phys. Rev. B 73 233403
[47] Rodriguez-Manzo J A, Lopez-Urías F, Terrones M and Terrones H 2004 Nano Lett. 4 2179
[48] Su H B, Nielsen R J, van Duin A C T and Goddard W A 2007 Phys. Rev. B 75 134107
[49] Zhu X and Su H B 2009 Phys. Rev. B 79 165401
[50] Rao S S, Stesmans A, Kosynkin D V, Higginbotham A and Tour J M 2010 arXiv:1006.4942v1
[51] Lee D W, Cole J M, Seo J W, Saxena S S, Barnes C H W, Chia E E M and Panagopoulos C 2010 arXiv:1005.5580v1
[52] Alexandre S S, Mazzoni M S C and Chacham H 2008 Phys. Rev. Lett. 100 146801
Magnetism in graphene oxide

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Abstract. The magnetic properties of graphene oxide have been investigated using spin-polarized density functional theory. A series of structures with an epoxy-pair chain at various positions on zigzag graphene nanoribbons is considered. The results show that this kind of graphene oxide is ferromagnetic at the ground state, providing great promise in the field of spintronics. In comparison with zigzag graphene nanoribbons of the same width, this graphene oxide is metallic and its spin density distribution is modified by epoxy pairs at different locations, thus rendering some fundamental insights into graphene-based materials.

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1. Introduction

Graphene, a two-dimensional single layer of graphite, became the subject of significant research efforts [1] immediately after the first report by Novoselov et al in 2004 [2, 3]. Graphene possesses novel electronic properties, including near-ballistic transport [2], massless Dirac fermions [4], Berry’s phase [5], the quantum Hall effect [4, 5] and high mobility [4], and it shows great promise for nanoelectronics [6]–[10]. Due to its optically transparent and conductive properties, graphene is also ideal for electrodes [11, 12] and photonics [13]–[16]. To enable various potential applications [17]–[21], it is important to modify graphene, including graphene nanoribbons [17], [22]–[24] and graphene-composed structures [25]–[28], to generate unique electronic properties.

To fabricate and/or modify graphene-based materials, oxidation has now become an important approach. For example, graphene can be cut into different sizes with oxygen plasma etching to produce nanoribbons [7] and quantum dots [29, 30]. In solution processing, graphene nanoribbons can also be generated by reducing graphene oxide [20]. Recently, graphene nanoribbons were even fabricated by unzipping carbon nanotubes (CNTs) with a simple oxidative process [31]. With an oxygen plasma treatment reported by Gokus et al [32], photoluminescence (PL) was first observed in single graphene layers.

With the oxidative process, graphene oxide exists widely as a critical intermediate during the fabrication and modification of graphene. It is fundamentally and practically valuable to study the electronic properties of graphene oxide and its incorporation into graphene layers, which could provide an atomistic understanding of the formation mechanisms for graphene and modified graphene materials. Based on first-principles study, several structures of graphene oxide [33, 34] have been proposed. Graphene is often functionalized by epoxy and hydroxyl groups during the fabrication and/or modification process. The epoxy groups have been suggested to align in a line on graphene or CNTs, and rupture carbon–carbon bonds to form ordered structures [33]. During the further oxidation process, the epoxy-pair structure is more favorable (a lower energy of 2.71 eV) rather than the scenario where an extra epoxy group is situated far from the existing epoxy chain [34]. It is also indicated [34] that only an energy of 0.1 eV is required to form one epoxy pair or add an epoxy group to extend the epoxy chain on graphene. It has been found that there is a high energy barrier of 0.76 eV [34] for the reaction of one epoxy pair to form one carbonyl pair, although the existence of one carbonyl pair is 0.45 eV lower than one epoxy pair [34]. Moreover, the energy barrier to break two neighboring epoxy pairs into two carbonyl pairs approaches 1.07 eV [34], indicating that the alignment of epoxy pairs on graphene could be a relatively stable state. It is possible to experimentally observe this state, because a similar graphene oxide has been found to be relatively stable, which can only become nanoribbons by sonochemical cutting [35].

Meanwhile, graphene nanoribbons, elongated strips of graphene with edges, sketch a different type of graphene structure [6, 22], [36]–[40]. The antiferromagnetic (AFM) property in zigzag graphene nanoribbons (ZGNR) [40] is particularly interesting among the magnetism in carbon materials. The confined ZGNR seems to possess magnetic properties. Some experimental work on the magnetism of oxidized graphene nanoribbons [50] and oxidized graphite [51] has been carried out very recently. One related study based on proposed CNTs with epoxy chains also represents magnetic properties [52]. Furthermore, some reports have shown that carbon-based structures could offer potential applications for spintronics [41, 42], including fullerene [43, 44], CNTs [45, 46] and hybrid carbon structures [47]–[49]. In this work, we perform theoretical
Table 1. Energy data of a set of n-ZGO-0 and n-ZGNR structures containing NM, FM and AFM states. Each total energy result is listed inside parentheses. The total energy differences of the NM and AFM states are compared with the corresponding FM ones. The total energy differences of ‘16-ZGO-random’ and ‘16-ZGO-⊥’ are compared with the NM state of 16-ZGO.

| Structure     | NM (meV unit cell⁻¹) | FM (meV unit cell⁻¹) | AFM (meV unit cell⁻¹) |
|---------------|----------------------|----------------------|-----------------------|
| 8-ZGO-0       | 53.9 (−3378074.9)    | 0.0 (−3378128.8)     | 15.7 (−3378113.1)     |
| 12-ZGO-0      | 51.8 (−4620068.2)    | 0.0 (−4620120.0)     | 7.0 (−4620113.0)      |
| 16-ZGO-0      | 57.7 (−5862022.3)    | 0.0 (−5862080.0)     | 6.6 (−5862073.4)      |
| 20-ZGO-0      | 60.1 (−7103982.8)    | 0.0 (−7104042.9)     | 5.9 (−7104037.0)      |
| 16-ZGO-random | 1352.8 (−5860669.5)  | – –                  | – –                   |
| 16-ZGO-⊥      | 1194.0 (−5860828.3)  | – –                  | – –                   |
| 12-ZGNR       | 47.4 (−3755969.3)    | 0.0 (−3756016.7)     | −3.2 (−3756019.9)     |
| 16-ZGNR       | 52.2 (−4997919.4)    | 0.0 (−4997971.6)     | −4.0 (−4997975.6)     |

studies of an epoxy-pair chain on zigzag graphene nanoribbons along the nanoribbon direction, particularly the magnetic properties of some unique graphene oxide structures, providing a family of graphene oxides as excellent candidates for magnetic nanoelectronics.

2. Results and discussion

To study the electronic properties of graphene oxide, we need to consider its stability. The total energies of the ordered epoxy-group structured graphene oxide and several structures with a random distribution of epoxy groups in graphene are calculated (see ‘16-ZGO-random’ in table 1), revealing that the latter has a higher energy than the former by ∼1.4 eV unit cell⁻¹. This indicates that a random structure is much less stable than an ordered one. Another structure of graphene oxide with an epoxy-group alignment in smaller chains perpendicular to the axis of the nanoribbon is also calculated, and is found to have higher energy than an ordered structure with the epoxy chain alignment along the nanoribbon direction by ∼1.2 eV unit cell⁻¹ (see ‘16-ZGO-⊥’ in table 1) and to have less stability than the latter. Thus, in this work we focus on the relatively stable structure, the ordered structure with the epoxy chain alignment along the nanoribbon direction.

The spin-polarized electronic structure of ZGNR with an epoxy-pair chain along the periodic direction is studied based on ab initio pseudopotential density functional theory (DFT) within the local density approximation (LDA) [53] by using the SIESTA package [54]. A double-ζ plus polarization basis set is employed for calculation. The energy cutoff for real-space mesh size is chosen as 300 Ryd. The initial structures are relaxed until the force on each atom is less than 0.04 eV Å⁻¹. The Monkhorst-Pack 41 × 1 × 1 k-point grid is chosen to sample the Brillouin zone (BZ). The unit length along the x-axis is 2.46 Å.

In accordance with the previous report [40], the classification of ZGNRs is defined by the number of zigzag chains ‘n’ to form the width, termed as ‘n-ZGNR’ (see the blue numbers in figure 1(a)). The positions for one epoxy pair per unit cell are labeled by blue dashed lines, and classified by the pink numbers ‘m’ to describe graphene oxide, finally termed as ‘n-ZGO-m’ in this paper (figure 1(b) and (c)). Here, we only discuss ZGOs, which contain even rings per
Figure 1. (a) Schematic illustrations of $n$-ZGNR, (b) $n$-ZGO-0 and (c) $n$-ZGO-1 from the top and side views. Orange balls denote hydrogen atoms, passivating the edge of the carbon atoms colored in gray. The oxygen atoms are illustrated in red. The green dashed rectangle denotes a single unit cell. Blue numbers 1–$n$ denote the width of the nanoribbons. Pink numbers 0–$m$ point out the positions of epoxy pairs during our studies.

unit cell labeled by a green dashed rectangle, obtaining maximum $m = n/4 - 1$. Thus, when an epoxy pair locates at the $m = 0$ position, the $n$-ZGO-0 also has a mirror plane (see the blue dashed line in figure 1(b)) compared with $n$-ZGNR.

The width ‘$n$’ and oxidation position ‘$m$’ are two main factors in ZGO. The width effect in ‘$n$-ZGO-0’-type structures is firstly studied. As a comparison, ‘$n$-ZGNR’ and ‘$n$-ZGO-0’, both processing mirror symmetries, are examined. Considering the spin polarization, the AFM, ferromagnetic (FM) and nonmagnetic (NM) configurations are considered to have favorable ground states. The energy data of the three configurations are listed in table 1. The energy differences of the AFM and NM states are compared with the corresponding FM states. In table 1, both 12-ZGNR and 16-ZGNR are AFM in terms of the reported results [22, 40], presenting a strong spin–orbital interaction. However, with the epoxy pairs, $n$-ZGO-0 devices exhibit FM states. The energy difference between non-spin-polarized and spin-polarized states is larger than 50 meV, and that between FM and AFM configurations is much smaller, decreasing as the width ‘$n$’ of graphene oxide increases. The energy differences between FM and AFM states per unit cell are 15.7, 7.0, 6.6 and 5.0 meV, for 8-ZGO-0, 12-ZGO, 16-ZGO and 20-ZGO, respectively.

Geometrical factors often determine the electronic properties. For further study, we compare the differences between 16-ZGNR and 16-ZGO-0 at first and then between 16-ZGO-$m$
Figure 2. (i) Electronic spin-polarized band structures, (ii) projected DOS and (iii) top- and side-view spin density plots of (a) 16-ZGNR, (b) 16-ZGO-0, (c) 16-ZGO-1, (d) 16-ZGO-2 and (e) 16-ZGO-3. In band structures, the majority-(up-) spin bands are plotted at the right parts with red, whereas the minority-(down-) spin bands are plotted at the left parts with black. The up (or down) pink arrows denote up- (or down-) spin bands. In projected DOS structures, the red (black) lines and blue (cyan) lines denote the majority- (minority-) spin projected DOS of whole devices and oxygen atoms, respectively. The Fermi energy is set to zero. Isosurfaces of spin density ($\pm 0.01 e \AA^{-3}$) are denoted by blue (positive) and red (negative) lobes. The positions of epoxy-pair chains are pointed out with red arrows.

structures. The spin-polarized band structures are first considered. Each band line is from $\Gamma (0, 0, 0)$ to $X (\pi/a, 0, 0)$ ($a$ is the unit cell length), as shown in figure 2. Thus, 16-ZGNR is a semiconductor and its direct band gap is 140 meV. In 16-ZGO-0, the band lines are 104 and 262 meV above the Fermi energy level in majority-spin and minority-spin segments, respectively, demonstrating a metallic property for 16-ZGO-0. In the isosurface of the spin density for 16-ZGNR, the majority and minority spins appear in two different sublattices, as shown in figure 2(a). Thus, a stronger AFM coupling exists in 16-ZGNR [40]. Evidently, the magnetic moment of each spin in each sublattice of 16-ZGNR is around 0.44 $\mu_B$, in agreement...
Table 2. Energy data of a set of 16-ZGO-$m$ ($m = 0, 1, 2$ and $3$) and 16-ZGNR structures containing NM, FM and AFM states. Each total energy result is listed inside parentheses. The total energy differences of the NM and AFM states are compared with the corresponding FM ones. Each total magnetic moment is listed as the value of the corresponding favorable ground state.

| Structure | NM (meV unit cell$^{-1}$) | FM (meV unit cell$^{-1}$) | AFM (meV unit cell$^{-1}$) |
|-----------|--------------------------|--------------------------|---------------------------|
| 16-ZGO-0  | 57.7 $(-5862022.3)$      | 0.0 $(-5862080.0)$       | 6.6 $(-5862073.4)$        |
| 16-ZGO-1  | 44.5 $(-5862029.8)$      | 0.0 $(-5862074.3)$       | 8.2 $(-5862066.1)$        |
| 16-ZGO-2  | 56.3 $(-5862002.9)$      | 0.0 $(-5862059.2)$       | 1.7 $(-5862057.5)$        |
| 16-ZGO-3  | 68.4 $(-5861897.5)$      | 0.0 $(-5861965.9)$       | 0.8 $(-5861965.1)$        |
| 16-ZGNR   | 52.2 $(-4997919.4)$      | 0.0 $(-4997971.6)$       | $-4.0$ $(-4997975.6)$     |

with the previous work [22]. However, in 16-ZGO-0, with the existence of oxygen atoms, the favorable ground state is FM; moreover, the large spin density locates at oxygen atoms, as shown in figure 2(b). The oxygen atoms divide ZGO into two parts. Each part could be considered as a ‘new’ zigzag graphene nanoribbon. Opposite spin states occupy different sublattices originating from staggered sublattice potentials [55, 56]. Then, in each part, the majority and minority spins also appear in two different sublattices. The magnetic moments of the majority and minority spins in their corresponding sublattice of each part are 0.60 $\mu_B$ and $-0.10$ $\mu_B$. Each oxygen atom contains a magnetic moment of 0.05 $\mu_B$.

In addition, with different epoxy-pair sites, a set of ‘16-ZGO-$m$’ is investigated. Regardless of 16-ZGO-0, other sites could break such a mirror symmetry shown in figure 1(b). The FM states are also favorable for their ground states obtained from the energy differences between FM, NM and AFM configurations (see table 2). Moreover, the energy difference between non-spin-polarized and spin-polarized states is still large, while the energy difference between FM and AFM configurations is much smaller. The energy differences between FM and AFM states per unit cell are 6.6, 8.2, 1.7 and 0.8 meV for 16-ZGO-0, 16-ZGO-1, 16-ZGO-2 and 16-ZGO-3, respectively. Comparing the FM energies in 16-ZGO-$m$ devices, 16-ZGO-0 is more stable.

The band lines near the Fermi level of the minority-spin part in figure 2(b) move upward as the epoxy-pair sites increase in (c)–(e). Meanwhile, from their projected density of states (DOS), the minority-spin peaks near the Fermi level have generally shrunk (see the black lines in figure 2(b)-(ii)–(e)-(ii)) while the contribution of oxygen atoms for projected DOS (see the blue and cyan lines in figure 2(b)-(ii)–(e)-(ii)) does not change too much. Thus, the different epoxy-pair site changes the spin density distribution of carbon atoms. Since the oxygen atoms divide the graphene nanoribbons into ‘upper’ and ‘bottom’ parts, the magnetic moments of the two parts are clearly not the same unless oxygen atoms locate at the middle. Obviously, the upper part of 16-ZGO-$m$ (except for 16-ZGO-0) gains more spin density distributions (see figures 2(c)–(e)), while the majority and minority spins appear in two different sublattices of each part as well. To clarify the trend from different epoxy-pair sites, the magnetic moments of majority and minority spins in the two parts are calculated, which can also be observed from the spin density isosurfaces in figure 2. In the upper part, the magnetic moment of the majority spin increases whereas the absolute value of the minority spin decreases as the site of the epoxy pair moves upwards. On the other hand, the trend is different in the bottom part. The oxygen atoms tend to gain more up-spins as their locations are closer to the upper edge.
Figure 3. (a) Structures of graphene. All bonds in graphene are equivalent, and the double bonds are marked for convenience of comparison with others. Structures of (b) zigzag edges passivated by hydrogen atoms and (c) oxygen atoms located in the zigzag direction of graphene. Schematic chemical forming: (e) C–H bonds and (f) C–O bonds from (d) graphene. The red and blue balls in (b) and (c) represent as $\alpha$-C and $\beta$-C atoms.

To consider the different magnetic configurations in ‘16-ZGNR’ and ‘16-ZGO-\textit{m}’, the magnetism from the orbitals’ hybridization is analyzed and estimated. First, two 2s and two 2p electrons in carbon atoms could form different sp-hybridized orbitals \cite{57}. In graphene, four orbitals of each carbon atom are hybridized to form sp$^2$ bonding, with its typical sp$^2$ C–C bond length of 1.42 Å. Meanwhile, three σ orbitals placed in the graphene plane with a value of 120° for the band angle, and one unpaired electron, are expected in the π orbital, which is along the $z$-axis in the perpendicular direction. Mostly, the process of breaking π bonds and producing new σ bonds results in the transformation of sp$^2$ hybridization to sp$^3$ hybridization, which is the mechanism of the magnetic properties in carbon nanostructures. Clearly, a change in bond length and angles exists in the transformation of sp$^2$ hybridization to sp$^3$ hybridization. For ideal sp$^3$ hybridization, the C–C bond length is 1.54 Å. The bond length between $\alpha$-C ($C_\alpha$) and $\beta$-C ($C_\beta$) atoms of graphene oxide in figures 3(c) and (f) is about 1.47 Å, between 1.42 and 1.54 Å. Then, an intermediate character of this hybridization is between sp$^2$ and sp$^3$. However, the net magnetic moment of $C_\alpha$ is nearly 0.00 in ZGO. Therefore, the hybridization of $C_\beta$ is sp$^2$ rather than sp$^3$ and the $C_\beta$ atom gains a larger net magnetic moment. On the other hand, in the ZGNR passivated by hydrogen atoms (see figures 3(b) and (e)), the bond between the $C_\alpha$ and $C_\beta$ atoms is 1.40 Å, resulting in sp$^2$ hybridization, and a larger net magnetic moment locates on $C_\alpha$ atom.

During the formation of graphene oxide in a solution process, KMnO$_4$/H$_2$SO$_4$ solution treatment to unzip CNTs has been reported by Kosynkin \textit{et al} \cite{31}. A recently published paper experimentally reveals paramagnetism in this kind of oxidized graphene nanoribbon \cite{50}, which is close to our proposed structure, thus supporting our calculations. The antiferromagnetism of...
one type of graphene oxide has been reported [51]. Since it has a structure different from our studied one, it is understandable that it exhibits different properties.

To experimentally realize the proposed structure in this work is also important. We choose 16-ZGO mainly with a width of $\sim 3.5$ nm, whose size can be experimentally realized in graphene. Moreover, the selectivity of the epoxy-pair chain position has many choices, since all ZGOs discussed here have FM properties. Once the epoxy chain exists, it is easy to form an epoxy pair or add a new epoxy group to extend the chain on graphene with an energy of 0.1 eV [34].

3. Summary

In conclusion, spin-polarized first-principles calculations of proposed graphene oxide structures have been conducted. A series of structures with the epoxy-pair chain at various positions on zigzag graphene nanoribbons is considered. This kind of graphene oxide is FM at the ground state, providing great promise in the field of spintronics. Moreover, with a comparison of the same width of ZGNR, ZGO is metallic. The spin density distribution can be modified with different sites of epoxy pairs. These discoveries can also render some fundamental insights into graphene materials.

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References

[1] Geim A K and Novoselov K S 2007 Nat. Mater. 6 183
[2] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666
[3] Novoselov K S, Jiang D, Schedin F, Booth T J, Khotkevich V V, Morozov S V and Geim A K 2005 Proc. Natl Acad. Sci. USA 102 10451
[4] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 Nature 438 197
[5] Zhang Y B, Tan Y W, Stormer H L and Kim P 2005 Nature 438 201
[6] Chen Z H, Lin Y M, Rooks M J and Avouris P 2007 Physica E 40 228
[7] Han M Y, Ozyilmaz B, Zhang Y B and Kim P 2007 Phys. Rev. Lett. 98 206805
[8] Katsnelson M I, Novoselov K S and Geim A K 2006 Nat. Phys. 2 620
[9] Lin Y M, Jenkins K A, Valdes-Garcia A, Small J P, Farmer D B and Avouris P 2009 Nano Lett. 9 422
[10] Feng X L, Chandrasekhar N, Su H B and Mullen K 2008 Nano Lett. 8 4259
[11] Kim K S, Zhao Y, Jang H, Lee S Y, Kim J M, Ahn J H, Kim P, Choi J Y and Hong B H 2009 Nature 457 706
[12] Eda G, Fanchini G and Chhowalla M 2008 Nat. Nanotechnol. 3 270
[13] Guo C X, Yang H B, Sheng Z M, Lu Z S, Song Q L and Li C M 2010 Angew Chem., Int. Ed. Engl. 49 3014
[14] Gusynin V P, Sharapov S G and Carbotte J P 2009 New J. Phys. 11 095013
[15] Hasan T, Sun Z P, Wang F Q, Bonaccorso F, Tan P H, Rozhin A G and Ferrari A C 2009 Adv. Mater. 21 3874
[16] Xia F N, Mueller T, Lin Y M, Valdes-Garcia A and Avouris P 2009 Nat. Nanotechnol. 4 839
[17] Biel B, Blase X, Trizion F and Roche S 2009 Phys. Rev. Lett. 102 096803
[18] Kamat P V 2010 J. Phys. Chem. Lett. 1 520
[19] Kan E J, Li Z Y, Yang J L and Hou J G 2008 J. Am. Chem. Soc. 130 4224
[20] Li X L, Wang X R, Zhang L, Lee S W and Dai H J 2008 Science 319 1229
[21] Yazhev O V and Helm L 2007 Phys. Rev. B 75 125408
[22] Son Y W, Cohen M L and Louie S G 2006 Nature 444 347
[23] Cresti A and Roche S 2009 New J. Phys. 11 095004
[24] Wakabayashi K, Takane Y, Yamamoto M and Sigrist M 2009 New J. Phys. 11 095016
[25] Stankovich S, Dikin D A, Dommett G H B, Kohlhaas K A, Zimny E J, Stach E A, Piner R D, Nguyen S T and Ruoff R S 2006 Nature 442 282
[26] Stankovich S, Dikin D A, Kohlhaas K A, Kleinhammes A, Jia Y, Wu Y, Nguyen S T and Ruoff R S 2007 Carbon 45 1558
[27] Furst J A, Pedersen J G, Flindt C, Mortensen N A, Brandbyge M, Pedersen T G and Jauho A P 2009 New J. Phys. 11 095020
[28] Heiskanen H P, Manninen M and Akola J 2008 New J. Phys. 10 103015
[29] Ponomarenko L A, Schedin F, Katsnelson M I, Yang R, Hill E W, Novoselov K S and Geim A K 2008 Science 320 356
[30] Trauzettel B, Bulaev D V, Loss D and Burkard G 2007 Nat. Phys. 3 192
[31] Kosynkin D V, Higginbotham A, Sinitskii A, Lomeda J R, Dimiev A, Price B K and Tour J M 2009 Nature 458 872
[32] Gokus T, Nair R R, Bonetti A, Bohmier M, Novoselov K S, Geim A K, Ferrari A C and Hartsuch A 2009 ACS Nano 3 3963
[33] Li J-L, Kudin K N, McAllister M J, Prud’homme R K, Aksay I A and Car R 2006 Phys. Rev. Lett. 96 176101
[34] Li Z Y, Zhang W H, Luo Y, Yang J L and Hou J G 2009 J. Am. Chem. Soc. 131 6320
[35] Wu Z S, Ren W C, Gao L B, Liu B L, Zhao J P and Cheng H M 2010 Nano Res. 3 16
[36] Cicero G, Grossman J C, Schwegler E, Gygi F and Galli G 2008 J. Am. Chem. Soc. 130 1871
[37] Wang Z F, Li Q X, Zheng H X, Ren H, Su H B, Shi Q W and Chen J 2007 Phys. Rev. B 75 113406
[38] Wu S D, Jing L, Li Q X, Shi Q W, Chen J, Su H B, Wang X P and Yang J L 2008 Phys. Rev. B 77 195411
[39] Son Y W, Cohen M L and Louie S G 2006 Phys. Rev. Lett. 97 216803
[40] Rao S S, Stesmans A, Kosynkin D V, Higginbotham A and Tour J M 2010 arXiv:1006.4942v1
[41] Lee D W, Cole J M, Seo J W, Saxena S S, Barnes C H W, Chia E E M and Panagopoulos C 2010 arXiv:1005.5580v1
[42] Alexandre S S, Mazzoni M S C and Chacham H 2008 Phys. Rev. Lett. 100 146801
[43] Wolf S A, Awschalom D D, Buhrman R A, Daughton J M, von Molnar S, Roukes M L, Chtchelkanova A Y and Treger D M 2001 Science 294 1488
[44] Zutic I, Fabian J and Das Sarma S 2004 Rev. Mod. Phys. 76 323
[45] Makarova T L, Sundqvist B, Hohne R, Esquinazi P, Kopelevich Y, Scharff P, Davydkov V A, Kashevarova L S and Rakhmanina A V 2001 Nature 413 716
[46] Hohne R and Esquinazi P 2002 Adv. Mater. 14 753
[47] Sahoo S, Kontos T, Furer J, Hoffmann C, Graber M, Cottet A and Schonenberger C 2005 Nat. Phys. 1 99
[48] Tombros N, van der Molen S J and van Wees B J 2006 Phys. Rev. B 73 233403
[49] Rodriguez-Manzo J A, Lopez-Urías F, Terrones M and Terrones H 2004 Nano Lett. 4 2179
[50] Su H B, Nielsen R J, van Duijn A C T and Goddard W A 2007 Phys. Rev. B 75 134107
[51] Zhu X and Su H B 2009 Phys. Rev. B 79 165401
[52] Troullier N and Martins J L 1991 Phys. Rev. B 43 1993
[53] Soler J M, Artacho E, Gale J D, Garcia A, Junquera J, Ordejon P and Sanchez-Portal D 2002 J. Phys.: Condens. Matter 14 2745
[54] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801
[55] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146802
[56] Pauling L 1932 J. Am. Chem. Soc. 54 3570

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