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Tremendous Spin-Splitting Effects in Open Boron Nitride Nanotubes: Application to Nanoscale Spintronic Devices

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Abstract: Our calculations demonstrate that the intrinsic magnetism of boron nitride nanotubes (BNNTs) can be induced by their open ends, and the resulting magnetic moment is sensitive to the chirality of BNNTs. It is found that BNNTs, a pure sp-electron system, present a tremendous spin-splitting larger than 1 eV and that B-rich-ended and N-rich-ended BNNTs exhibit "conjugate", spin-polarized, deep-gap states. Tremendous spin-splitting effects combined with considerable local spin-polarizations at the open ends make BNNTs significant for applications of nanoscale spintronics such as spin-polarized electron emitters.

I. Introduction

Spintronics, which uses electron spin instead of its charge as the information carrier, is igniting a revolution in computer science, information science, and many other areas.[1] It is predicted, on the basis of each spin carrying a bit of information, that the single-spin transistors will not only lead to faster computers that consume less electricity but also alleviate the problem of heat dissipation. In designing spintronic devices, much effort has been directed toward the doping of transition-metal atoms into II−VI or III−V semiconductors to fabricate ferromagnetic nanostructures.[2] Recently, nanotubes (NTs) are confirmed to offer exciting opportunities in the fabrication of spintronic devices due to their unique hollow tubular structures and fantastic chemical and physical properties.[3] It has been shown that NTs doped with some foreign atoms, such as alkali metal[3] and 3d transition-metal atoms[4] may exhibit room-temperature ferromagnetism. However, problems with compatibility and bonding between the host and the metal dopants may arise, which would have crucial effects on the qualities and properties of these hybrid nanostructures. This has provoked much speculation in the area of inducing magnetic properties of NTs by artificial means.

Boron nitride nanotubes (BNNTs), a conventional representation of one-dimensional (1-D) III−V compounds, have a uniformly wide band gap[5] and high chemical stability,[6] which ensure them to be used as "host" and "mold" for growing nanocrystals and nanowires.[7] Ab initio molecular dynamics simulations showed that the growth mechanism and closure behavior of single-walled BNNTs are strongly dependent on their chiralities,[8] whereas open BNNTs have been unambiguously observed or artificially fabricated experimentally.[9] Compared with CNTs, BNNTs might be more suitable for the study of the quantum behaviors of s and p electrons under quantum confinement (i.e., surface or boundary), because they do not have the *delocalized* π electrons. In this work, we explore the effects of the open ends on the intrinsic magnetism of BNNTs using first-principles calculations. We first investigate the interaction between the atoms at the mouth and the spin configuration of unpaired electrons. Then we comparatively address the issues of the magnetic moments and spin-splitting effects of open B-rich-ended and N-rich-ended ones. We quantitatively analyze the spin-polarized electronic structures and general chirality-dependent magnetic properties of open BNNTs and explore the stability of the local spin configuration of the tube mouth under external perturbations. Our results suggest that open BNNTs have promising applications in future spintronic devices.

II. Models and Method

In this work, a series of finite-length BN cages with different chiralities are adapted to model single-walled open (*n*,*m*) BNNTs, where one mouth is opened and the other is saturated by H atoms to represent the half-infinite boundary conditions (Figure 1). The lengths of the finite tubes used are 9.9−12.7 Å, i.e., 12 atomic layers for (6,3) BNNT, 13 atomic layers for (7,4), (8,0), and (9,0) BNNTs, and 8 atomic layers for (5,5) BNNT. The diameters are around 6.4−8.0 Å. For each kind

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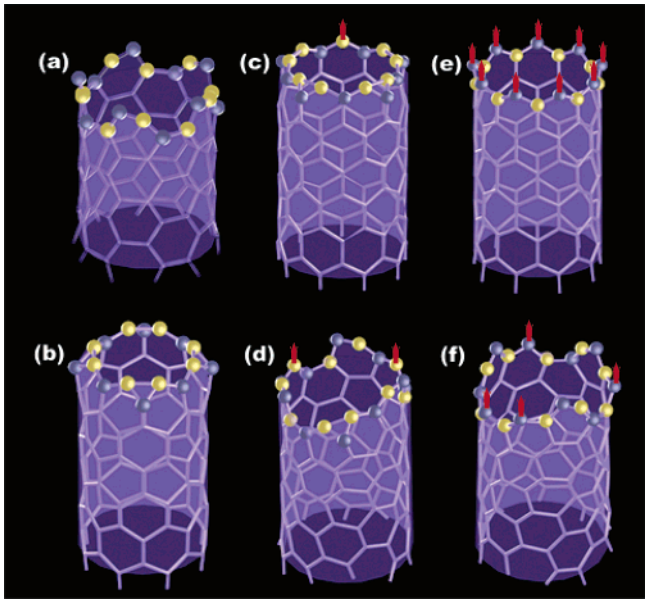

Figure 1. Optimized geometrical structures and ground-state spin configurations at the mouth of open BNNTs: (a) (5,5); B-rich-ended (b) (8,0), (c) (9,0), and (d) (7,3); N-rich-ended (e) (9,0), and (f) (7,3). To illustrate the mouth configurations more clearly, only the first two layer atoms at the open ends are shown, and the tube bodies are represented by meshes. The yellow and blue balls represent, respectively, B and N atoms. H-atom termination at the other end of the tube is not shown.

of open (*n*,*m*) tube, the numbers of atoms are the same for B-rich-ended and N-rich-ended models.

Using the DMol[3] package,[10] we carry out structural optimizations and total-energy calculations within the spin-polarized density functional formalism. The generalized gradient approximation combining the Perdew−Wang correlation functional[11] with the Becke exchange functional[12] is utilized. The double numeric polarized basis sets are utilized. Structural optimizations are deemed sufficiently converged when the forces on all ions are less than 10^{-3} au.

III. Results and Discussion

In principle, the atomic configuration of the mouth of any open BNNT is characterized by the B−N pairs or isolated B (N) atoms. Initially, each atom (B or N) at the open end has one unpaired electron, corresponding to one dangling bond, just as in open CNTs;[13,14] however, after structural relaxations, the configuration of the tube mouth changes a lot (as shown in Figure 1) due to the interaction between the neighboring atoms. Typically, for the open (5,5) BNNT, only 5 B−N pairs are presented at the mouth. The charge transfer on each B−N pair is up to 0.115 e, a bit larger than that on the body (0.100 e). This increase of ionicities of the B and N atoms at the mouth further strengthens the B−N pair bonding (demonstrated by the charge density difference shown in Figure 2a), and decreases the bond length from 1.45 to 1.31 Å. The in situ hexagonal rings are greatly buckled (Figure 1a). In open B-rich-ended (8,0), (9,0), and (7,3) BNNTs, the mouths undergo a Jahn−Teller distortion. The nearest two B atoms dimerize spontaneously, leading to a weak B−B bond with the length of 1.63−1.65 Å

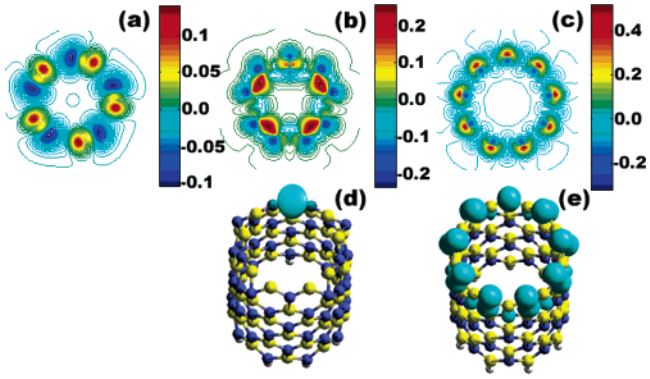

Figure 2. Contour plots of charge density difference [in units of e/(au)^3] at the open mouth of (a) (5,5), (b) B-rich-ended (9,0), (c) N-rich-ended (9,0) BNNTs, and spin density of (d) B-rich-ended (9,0) and (e) N-rich-ended (9,0) BNNTs.

(Figure 2b). As a result, BBN triangles are formed at the mouth (b, c, and d of Figure 1). This B−B dimerization was first observed by Blase et al. in their study on the growth mechanism of BNNTs.[8] Furthermore, the open B-rich-ended (8,0) tube spontaneously closes its mouth due to the perfect B−B dimerizations (i.e., 4 B−B dimers), while at the mouth of (9,0) tube there is one isolated B atom left with a little shift inward radially after the B−B dimerizations. On the contrary, at the ends of open N-rich-ended (8,0), (9,0), and (7,3) tubes, the repulsion between localized p_z electron states of N atoms prevents the unpaired electrons of two neighboring N atoms from bonding (Figure 2c). As a result, all N atoms at the open end shift away radially, leading to a slightly broader opening of the tube mouth (e and f of Figure 1). Our calculation results show that the B-rich-ended open tubes have higher binding energies (more stable) than the N-rich-ended ones.

Our calculations demonstrate that the spin configuration is dominated by the atomic configuration of the tube mouth in the open BNNT. In detail, for one B−N pair at the mouth, because of the large overlap between the electron clouds of the B and N atoms, the spin configuration of the nearest two unpaired electrons is antiparallel, following the Pauli exclusion principle. Thus, the B−N pair never contributes to the magnetic moment, and all open armchair (*n*,*n*) BNNTs are still nonmagnetic (Figure 1a). On the other hand, compared to the cases in open zigzag CNTs,[13] the spintronic behaviors in open zigzag BNNTs are much more complicated because they consist of two constituents and have two distinctly different atom terminations at the open ends. In open B-rich-ended BNNTs, the weak B−B dimerization effectively "saturates" the original dangling bonds of the nearest two B atoms, and the corresponding electrons are spin-antiparallel, obeying the Pauli principle (Figure 2d). As expected, the formation of B−B pairs does not introduce any magnetic moment to the system, and the unpaired electrons of the unpaired B atoms are spin-parallel, obeying Hund's rule. Thus, the open B-rich-ended (8,0) tube is nonmagnetic as is the (5,5) one, while the (9,0) tube has 1 μ_B net magnetic moment (as shown in b and c of Figure 1). However, in open N-rich-ended tubes, the spin-parallel configuration of unpaired electrons of the N atoms is energetically favorable (Figure 1e), abiding well by the Hund's rule. Thus, the obtained magnetic moment is equal to the number of unpaired electrons or dangling bonds (Figure 2e) as in the case of open zigzag CNTs.[13]

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Table 1. Atomic Configuration (Numbers of B−N Pairs, B−B Pairs, Unpaired B and N Atoms) and the Magnetic Moment of the Open End of the (*n*,*m*) BNNT; Mouth of (5,5) Tube Consists of Only Five B−N Pairs with 0 Magnetic Moment

	B-rich-ended				N-rich-ended		
chirality (*n*,*m*)	B–N	B–B	B	mag. (μ_B)	B–N	N	mag. (μ_B)
(8,0)	0	4	0	0	0	8	8
(9,0)	0	4	1	1	0	9	9
(6,3)	3	0	3	3	3	3	3
(7,3)	3	1	2	2	3	4	4

In the following, we probe the physical mechanism governing the chirality-dependent magnetic properties of open (*n*,*m*) BNNTs through analyzing the atomic and spin configurations. For an open (*n*,*m*) BNNT, the open mouth consists of *m* B−N pairs and $|n - m|$ isolated B (N) atoms. Our investigations confirm three basic features of the atomic configuration and the spin-pairing mechanism of the optimized tube mouth: (1) if the two nearest neighbor atoms at the mouth are not of the same type, two unpaired electrons from this B−N pair form one spin-antiparallel pair; (2) if the two nearest neighbors are the B atoms, no magnetic moment is introduced due to the weak B−B dimerization; (3) if the two nearest neighbors are the N atoms, each N atom will supply one magnetic moment because the unpaired electron located at each N atom is strictly isolated. Thus, in any open (*n*,*m*) BNNT the magnetic moment, which originates from the unpaired electrons, could be immediately evaluated from the number of unpaired B (N) atoms at the open mouths. For an open (*n*,*m*) BNNT, it is reasonable to assume that the cross section of the opening is as vertical to the tube axis as possible (i.e., the B−N pairs and the isolated B (N) atoms are spread alternately, at the most optimum), according to the experimental fact that NTs grow uniformly in the fabrication. As a result, a fundamental correlation between the chirality and magnetic moment M (μ_B) can be deduced as:

$$M = \begin{cases} n - m, & \text{N rich} \\ \begin{cases} k, & l = \text{even}, \\ m - k, & l = \text{odd}, \\ \text{mod}(n,2), & m = 0, \end{cases} & \text{B rich} \end{cases}$$

where l and k are, respectively, the quotient and the remainder of the integer division of $(n - m)$ by m (without loss of generality, we assume $n \geq m$). This correlation is clearly verified by our first-principles calculations of the optimized atomic and ground-state spin configurations (Figure 1) and the computed magnetic moments (listed in Table 1) for various BNNTs [armchair (5,5), zigzag (8,0) and (9,0), and chiral (6,3) and (7,3) BNNTs].

The previous study showed that the electronic property of the (*n*,*m*) BNNT is not sensitive to its chirality,[5] impeding its application potential in *nanoelectronic* devices, whereas the present finding that the magnetic property of the open (*n*,*m*) BNNT depends on the chirality might effectively promote its practical application in *nanospintronic* devices. Typically, open (*n*,*m*) BNNTs could be used as the magnetic microscopy tips. It is significant that the BNNT tips without any magnetic atom doping could exhibit plentiful chirality-dependent magnetic properties. Furthermore, the atomic configuration of the open end and the chirality of the open (*n*,*m*) BNNT might be precisely

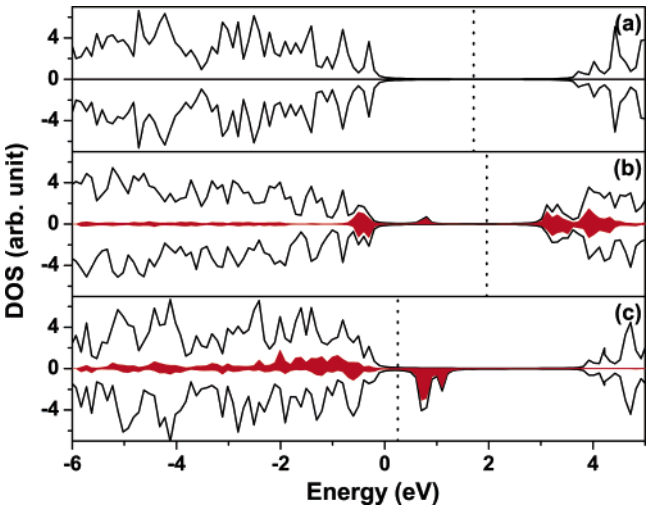

Figure 3. Density of states of (a) closed, (b) B-rich-ended, and (c) N-rich-ended open (9,0) BNNTs. Dotted line indicates the Fermi level. Here, the energy zero is shifted for the convenience of comparison. The red area corresponds to LDOS of the atoms at the mouth.

detected from the measured spin-polarized electron energy distribution or pattern. This probably prefigures a new nanometer-measuring and -testing technique.

Generally, in the open-shell systems, the unpaired valence electrons will result in spin-splitting of the highest occupied molecular orbitals (HOMOs) of the different spin components. For example, different from the closed (9,0) BNNT (a closed-shell system) with both ends terminated by H atoms, the open (9,0) BNNT (an open-shell system) exhibits spin-polarized states in the gaps due to their intrinsic local magnetism, as shown in Figure 3. For the open B-rich-ended (9,0) tube, there exists one occupied gap state of *majority* spin, whereas in the open N-rich-ended (9,0) tube, nine unoccupied gap states of *minority* spin appear. Local density of states (LDOS) of the tube mouth (the red areas of b and c of Figure 3) and the molecular orbital analysis[14] demonstrate that, in open BNNTs, the spin-polarized gap states mostly originate from the unpaired B or N atoms at the open ends. In the open B-rich-ended (9,0) tube, the unpaired electron bound by the unpaired B atom is responsible for the spin-polarized occupied state of majority spin, as shown in Figure 3b. At the N-rich end of the open (9,0) tube, the spins of unpaired electrons are parallel, and these electrons occupy the deeper states under HOMO level with majority spin, and then, the same number of unoccupied states of minority spin are left in the gap, as shown in Figure 3c. It is interesting to note that the spin-polarized gap states are occupied for the B-rich-ended (9,0) BNNT, but unoccupied for the N-rich-ended tube. This difference of the gap states originates from the different local potentials in the vicinities of the different open ends, similar to the cases of the gap states induced by III group and V group vacancies in bulk III−V semiconductors.[15−18]

From Figure 3, we can also find that two kinds of open BNNTs exhibit distinctly different tremendous spin-splitting effects in the gap. In the open B-rich-ended (9,0) tube, the existence of a polarized, occupied, deep-gap state results in an energy difference of 1.2 eV between the HOMOs of the majority spin and minority spin, whereas in the open N-rich-ended (9,0) tube, the nine polarized, unoccupied, deep-gap states lead to an energy difference of 3.25 eV between the lowest unoccupied molecular orbitals (LUMOs) of the majority spin and minority

spin. More generally, the spin-polarized, deep-gap states and similar enormous spin-splitting behaviors are also observed in open (6,3), (7,3), and N-rich-ended (8,0) tubes. In the B-rich-ended cases, the energy differences between majority- and minority-spin HOMOs are 1.49 and 1.17 eV for open (6,3) and (7,3) tubes, respectively, while in the N-rich-ended cases, the energy differences between majority- and minority-spin LUMOs are 3.23, 3.37, and 3.01 eV respectively for (6,3), (7,3), and (8,0) tubes. It should be noted that in open BNNTs, the gap states appear to be "conjugate": in the B-rich-ended ones, the gap states are occupied in the majority spin, while in the N-rich-ended ones, the gap states are unoccupied in the minority spin. Previously, Kim et al.[13] have theoretically demonstrated that partly opened intermediate carbon cage structures (such as the C_{60} fullerene and zigzag CNTs), typical open-shell systems, may induce the local magnetic moment. However, our calculations show that the spin-splitting effect in open CNTs is much weaker than those in open BNNTs (for example, the calculated spin-splitting in open (8,0) CNT is only 0.32 eV), consistent with the fact that CNTs have much smaller band gaps than BNNTs.[19] Moreover, our calculations for open (7,3) CNT show that the "antiferromagnetic" spin configuration (four dangling bonds with 2 spin-up, 2 spin-down) of the tube end is energetically preferred, leading to zero total magnetic moment of the system. Evidently, different open CNTs could have very different magnetic properties at the open tube ends. With large spin-splitting and uniform magnetic properties, open BNNTs would be more suitable to applications in nanospintronic devices than open CNTs.

It is important to understand the intrinsic origin of the large spin-splitting in open BNNTs. In covalent semiconductor crystals, lattice defects such as vacancies are well-known to produce the deep-gap states because the breaking of covalent bonds leads to a strong perturbation of the valence charge distribution.[16] Similarly, the open ends of BNNTs, as a kind of lattice defect, also introduce the deep defect states in the pristine gap. Moreover, since the local magnetism of the open tubes is also induced by the open ends, all those deep-gap states induced by the open ends are spin-polarized. For example, from the orbital distribution analysis for the B-rich-ended open (9,0) BNNT, we can see that the HOMO of the majority spin is mainly contributed by the unpaired B atom with a dangling bond at the open mouth, corresponding to a spin-polarized, deep-gap state, while the HOMO of the minority spin is mainly contributed by the B−B dimer, corresponding to a usual bonding state. With quite different bonding characteristics, these two HOMO states of different spin components are very different in energy (i.e., one is the deep-gap state, and the other is not), leading to a large spin-splitting between them. Therefore, the large spin-splitting in open BNNTs results from: (i) different bonding characteristic of the HOMOs of different spins and/or (ii) the appearance of spin-polarized, deep-gap states. In essence, this kind of splitting is different from the (conventional) large splitting induced by a large exchange-correlation interaction of magnetic atoms.

For practical spintronic devices, it is crucial to realize continuous and efficient emission of the spin-polarized electron current/beam at room temperature. Traditionally, the spin-polarized electron beams are obtained with the use of optical techniques in which the circularly polarized photons transfer their angular momenta to the electrons of semiconductor photocathodes, such as GaAs. Due to its specific band structure and the restriction of selection rules, the maximum theoretical spin-polarization in GaAs is only 0.5.[20] On the basis of the electron emission characteristics of 1-D nanosystems,[21] we have proposed to fabricate the spin-polarized electron emitters using 1-D nanostructural materials doped with the transition-metal atoms.[22] Alternatively, our present finding reveals that a novel spin-polarized electron emitter in cold cathode emission can be designed on the basis of using its own s, p electrons. Since no doping is needed in this design, the problems of compatibility and bonding between the foreign atoms and host lattice are completely avoided. Especially in the open B-rich-ended BNNT, the induced spin-polarized deep-gap states, corresponding to the tremendous spin-splitting of the HOMOs, are localized at the open-end, where a huge local electronic field induced by the high curvature of the mouth is accumulated. This means that a spin-polarized electron current/beam might be easily extracted under the relatively low operating voltage (corresponding to cold cathode emission). The spin-polarizations P of open BNNTs are evaluated through the LDOS.[22] In the N-rich-ended cases, the spin-splittings of HOMOs are very weak, corresponding to the small spin-polarizations. The spin-polarization of the open N-rich-ended (9,0) tube, for example, is lower than 0.33 within 3.0 eV below the Fermi level. On the contrary, the estimated maximum spin-polarizations (P_{max}) of open B-rich-ended (6,3), (7,3), and (9,0) tubes are, respectively, 0.96, 0.92, and 0.86, much higher than the values of the Mn-doped GaN NTs.[22] Furthermore, for open B-rich-ended BNNTs, the greater the magnetic moment is, the larger the P_{max} is.

In what follows, we will study the stability of the local spin configuration of the open tube end under external perturbations (electric field, doping, and interaction with the sample), which is crucial for practical nanoscale spintronics applications of BNNTs. First, as an example, we will discuss in detail the behavior of the two kinds of zigzag (9,0) open BNNTs under an external electric field. We find that the local magnetic

(15) In general, an open end in nanotubes can be regarded as a structural defect. Although it is well-known that the structural defects such as vacancies in covalent semiconductors will lead to deep gap states, the types (occupied or unoccupied) and accurate positions of these deep states can hardly be deduced directly from straightforward phenomenological physical models, since different defects often induce very different localized potentials.[16] However, some qualitative rules have been concluded by previous works.[17] It is found that the two kinds of vacancies (III group vacancies and V group vacancies) in III−V semiconductors result in very different localized potentials (weaker and stronger) in the vicinities of the defects. This further leads to their very different roles: III group vacancies behave as acceptors, and V group vacancies, as donors.[18] For open III−V nanotubes, the open ends could be regarded as structural defects (e.g., the B-rich open end as N vacancies, and the N-rich open end as B vacancies). Our calculation results also follow the above qualitative rule, that is, in the B-rich-ended (corresponding to N vacancies) BNNTs, the gap states are occupied (donorlike), while in the N-rich-ended ones (corresponding to B vacancies), they are unoccupied (acceptorlike).

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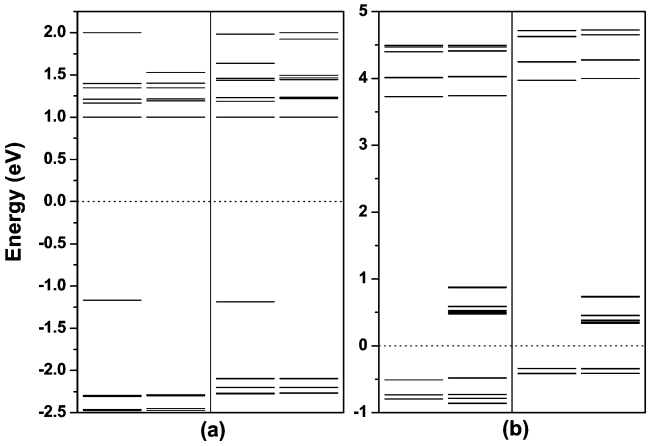

Figure 4. Energy spectrums of (a) B-rich-ended and (b) N-rich-ended open zigzag (9,0) BNNTs under electric field of 0 (left) and 0.1 V/Å (right). The Fermi level is set to zero.

property (i.e., local spin configuration) is not affected by the strong external field (up to 0.26 V/Å), and the magnetic moments of the open end of all tubes studied remain unchanged with the change of the field strength. On the other hand, the spin-splitting of B-rich-ended open (9,0) BNNT is reduced with an enhanced field. Such a reduction, however, is not significant. When the electric field is as large as 0.1 V/Å, the energy difference between the HOMOs of majority spin and minority spin is 0.9 eV, only 0.22 eV smaller than that under zero field (as shown in Figure 4a). It should be noted that 0.1 V/Å is truly a very strong electric field, about 40 times larger than the turn-on field for field emission of BNNTs (In the field emission of BNNTs, the turn-on field is about 0.0025 V/Å, i.e., 150 V bias with 6 μm between the tube tip and another electrode[23]). Under an electric field of 0.1 V/Å (minus bias), the spin-polarized gap levels of N-rich-ended open (9,0) BNNT shift down by 0.39 eV compared with that under zero field (as shown in Figure 4b). Meanwhile, the spin-polarized gap states are still mainly contributed by the unpaired atoms at the open end and remain unchanged under such a strong electric field. In a word, a strong electric field does not lead to the substantial changes of the local magnetic moment and the spatial distribution of the spin-polarized gap states, but will induce the changes of the energy gap and the spin-splitting effect. This indicates that the open BNNTs could be a good candidate for the spin-polarized electron emitters in wide applications.

Along with the fascinating development of the scanning tunneling microscope (STM), spin-polarized or magnetic tips are employed to probe the real-space magnetic structures down to the atomic scale,[24] and the spin-polarized scanning tunneling microscope (SP-STM) has attracted much attention for high-resolution surface magnetic imaging techniques. As shown in Figure 5, the spin-polarized electrons from the BNNT tip can pass through the barrier to fill the spin-polarized empty surface states on the sample, when the spin-polarized tip electron states and the empty surface states are aligned at the same level at an external bias. With a definite bias condition, the magnetic imaging of a surface can be illustrated at atomic scale through the variation of the tunneling current. On the basis of this idea,

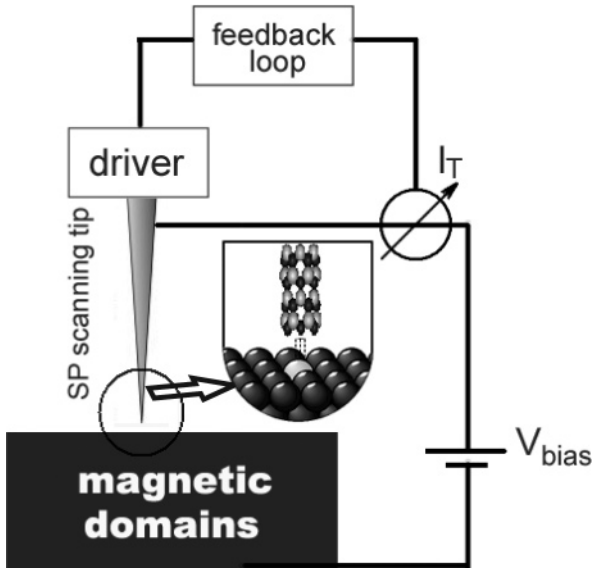

Figure 5. Scheme of a spin-polarized scanning tunneling microscope using an open BNNT tip.

we also study the effect of the interaction between the BNNT tip and the sample, which is critical to the practical applications in SP-STM. We set up a simplified model by taking the N-rich-ended open (9,0) BNNT as the tip of SP-STM, and a triangle formed by three iron atoms as the sample. The distance between the tube end and the triangle is taken to be around 1 nm which is the typical distance between the STM tip and the sample (noncontact mode; see, for example[25]). Our calculations show that the "ferromagnetic" spin configuration of the BNNT tip remains unchanged and is independent of the spin direction of the sample (three iron atoms). Therefore, the stability of local spin states of the tip (the tube end) is kept when interacting with magnetic samples.

Moreover, in practical application of BNNT, doping is an efficient method to improve its conductivity property. For example, in experiments, it is convenient to realize the functional doping of C atoms into BNNTs.[26] Here, we explore the doping effect by substituting B or N atoms at the tube body near the open ends (not at the open ends) by C atoms. Our results show that for both B-rich-ended and N-rich-ended open zigzag (9,0) BNNTs, the spin configuration will not be broken by C substituting either B or N atoms at the tube body near the open ends, or even by C substituting a B−N−B−N··· atom wire throughout the tube body. This confirms the stability of local spin states under C doping at the tube body. Actually, our calculation results show that the variation of electronic structure of the tube body will hardly affect the local magnetic property (spin configuration) of the open tube mouth. Meanwhile, our additional calculations performed on carbon-doped open (9,0) BNNTs show that the wide energy gap is effectively narrowed. And it has been reported that in the $B_XC_YN_Z$ nanotubes, the energy gap is much smaller than that of the BNNTs.[27] Moreover, as the transport property of the tube body is improved by doping, the spin-splitting induced by the open tube mouth (the emission

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zone) is found to be only slightly influenced (e.g. still 1.13 eV for the case of substituting a B−N−B−N··· wire by carbon atoms in B-rich-ended open (9,0) BNNT). Thus, the high spin-polarization of the tube mouth would be still kept, which ensures efficient emission of the spin-polarized electrons.

IV. Summary

In summary, by first-principles calculations, we elucidate the geometrical, magnetic, and electronic structures of a series of open BNNTs with different chiralities. Tremendous spin-splitting (>1 eV) in such a pure sp-electron system are first observed with the appearance of "conjugate", spin-polarized, deep-gap states. It is found that the chirality determines the atomic configuration of the mouth, the magnetic character (local magnetic moment), and spin-polarized electronic structure (energy gap and spin-splitting of HOMO states) of the open BNNT. The unpaired electrons of unpaired atoms at the mouth are responsible for the local magnetic moment and the spin-polarized, deep-gap states. Local spin configuration at the tube mouth is found to be stable under the external perturbations (such as strong electric field, doping at the tube body, and interaction with ferromagnetic samples). High spin-polarizations of open B-rich-ended BNNTs, combined with the high stability of their local spin configuration, indicate that they could be used as the promising candidates for nanoscale spin-polarized electron sources in future spintronic devices (such as spin-polarized electron field emitters and SP-STM tips). The spin-polarized electrons might also be emitted from open N-rich-ended BNNTs under near-infrared photon assistance. It is the interaction between the atoms at the mouth that determines the spin configuration of unpaired electrons and their different contributions to the intrinsic magnetism of the open BNNT. This mechanism might be general for other open III−V semiconducting NTs and nanowires (NWs) (such as open GaN NTs or NWs) due to their similar bonding characteristics. It is also possible that the analogous intrinsic magnetism might be presented in open II−VI semiconducting nanostructures. This, however, requires more in-depth investigations in the future.

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