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Electronic and magnetic properties of graphene Möbius strips: Density functional theory approach

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Abstract: Electronic and magnetic properties of graphene Möbius strips with different widths are studied using density functional theory. It is shown that the multiplicity of the Möbius strip, the cohesive energy, and the band gap energy increase with increasing the width of Möbius strip. We show that the magnetic moment of Möbius strip decreases with increasing the curvature and strain. Then the effects of an external electric field applied in the direction of the Möbius strip axis are studied and it is found that the Möbius strip keeps its metallic surface (edge) states even in the presence of the electric field. For sufficiently high applied electric field, the spin-flipping can take place in the Möbius strip. In addition, in contrast with the graphene nanoribbons, the graphene Möbius strips show half-semiconducting properties when an external electric field is applied.

Keywords: Graphene Möbius Strips, Magnetic Moment, and Spin-Dependent Density of States

I. Introduction

The Möbius strip has only one side and can be considered as a meta-material [1]. It has a non-oriented surface and has interesting physical and optical properties [2-4]. A Möbius strip of a single $NbSe_3$ crystal has been fabricated by modifying the conventional growth conditions [5] and the Möbius aromatic hydrocarbon has been observed [6]. Since graphene has good elastic and mechanical properties [7], it can be considered as a promising material to build Möbius strips [8]. The zigzag-edged graphene nanoribbon has interesting electronic and spintronic properties such as localized edge states and anti-ferromagnetic ground state [9-12]. Since the spin-orbit coupling is small in graphene, observation of spin Hall effect is difficult [13]. But, it has been shown that the Möbius graphene has nontrivial properties although the spin-orbit coupling is small [14-16]. By using tight binding method, Guo *et al.* have shown that the zigzag-edged graphene Möbius strip is a topological insulator [17]. Topological insulators have remarkable physical properties and have potential applications in quantum computing and spintronics [18]. The effect of Möbius topology on the electronics properties of graphene nanoribbon rings has been studied [19]. Also, the effect of twisted angle on the electronic and magnetic properties of Möbius strips has been reported [20]. Wang *et al.* have investigated the deformation energy density and edge magnetism of different graphene Möbius strips [21].

In this paper, the electronic and magnetic properties of Möbius strips made of zigzag graphene nanoribbons are studied using density functional theory (DFT). Here, we want to study the effect of multiplicity, 2S+1 (S means spin), strain and curvature on the magnetic moment of carbon atoms of Möbius strips. Also, the effect of electric field on the electronic and magnetic properties of Möbius strips is studied. It is shown that the Möbius strip has stable configuration and its multiplicity (2S+1) and cohesive energy increase with increasing the width of Möbius strip. Also, we show that by increasing the width of the Möbius strip the band gap energy increases. The Möbius strip has ferromagnetic properties and the curvature and strain of Möbius strip affect its magnetic moment. Then, we show that the spin-dependent density of states at zero-energy is not zero for both spin up and spin down. The non-zero density of states is due to the non-zero surface (or edge) density of states. The effect of an external electric field on

Möbius strip is studied and it is shown that, for low electric field, the graphene Möbius strip sustains its metallic edge states. Also, the Möbius strip shows half-semiconducting properties in the presence of electric field. When the electric field exceeds a critical value, the spin flipping can take place in the Möbius strip. The paper is organized as follows. Section II contains the calculation method. The results are presented and discussed in Sec. III. Finally, a summary is given in Sec. IV.

2. Calculation Method

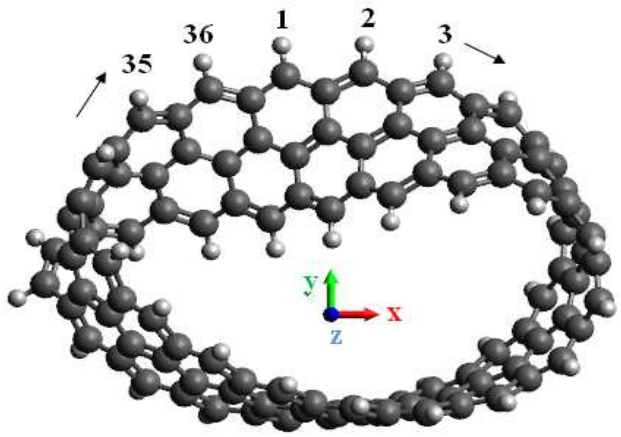


Fig 1. *(Color online) Zigzag-edged graphene Möbius strip with length L=18 and width N=3. The Möbius axis and edge carbon atom index are shown in the figure*

Consider a Möbius strip made of a zigzag graphene nanoribbon as shown in Fig. 1. We use DFT to relax the Möbius graphene strip (here we use Gaussian code [22]). The cohesive energy of graphene Möbius strips and graphene ribbons can be calculated by

$$E_{co}^{r(M)} = \frac{E_{SCF}^{r(M)} - N_C \times E_{SCF}^{C} - N_H \times E_{SCF}^{H}}{\sum (N_C + N_H)}. \qquad (1)$$

In Eq. (1), the superscript r(M) corresponds to the graphene ribbon (Möbius strip), N_C is the number of carbon atoms, N_H is the number of hydrogen atom, $E_{co}^{r(M)}$ is the self-consistent field energy of the graphene ribbon (Möbius strip), E_{SCF}^{C} and E_{SCF}^{H} are the self-consistent field energy of alone carbon and hydrogen atoms, respectively. Note that the cohesive energy of graphene ribbons is calculated for comparison.

Using local spin density approximation (LSDA), the local magnetic moment of carbon edge atoms is calculated. We use B3LYP functional [23-26] and 3-21G basis set [27, 28] because it has been shown that these basis set are suitable for carbon-based nano-structures [27, 28]. The difference between the lowest unoccupied molecular orbital (LUMO) energy and highest occupied molecular orbital (HOMO) energy is defined as band gap energy [22]. Using Gaussian code, the Fock and Overlap matrices of spin up and spin down electrons are calculated. The density of states (DOS) can be written as

$$DOS = \frac{-1}{\pi} Imaginary[Trace(G)] \qquad (2)$$

where

$$G = [Fock - (E + i\eta) \times Overlap]^{-1} \qquad (3)$$

is the Green function, E is the electron energy and η is an infinitesimal positive number. To calculate the effects of an external electric field on Möbius strip properties, we use the field command of Gaussian code [22] which is a perturbation method.

3. Results and Discussion

A graphene Möbius strip with length L=18, and width N=3, is shown in Figure 1. The Möbius axis and the edge carbon atom index are shown in the figure. The width of Möbius strip is defined as its number of zigzag strip. The *x, y, z* coordinates of Möbius strip are given by

$$x(u,\upsilon) = [r + \omega\upsilon \cos(u/2)]\cos u\,, \qquad (4)$$

$$y(u,\upsilon) = [r + \omega\upsilon \cos(u/2)]\sin u\,, \qquad (5)$$

$$z(u,\upsilon) = \omega\upsilon \sin(u/2)\,, \qquad (6)$$

where r and 2ω are the radius and width of the Möbius strip, respectively. In Eqs. (4) – (6), $0 \le u \le 2\pi$ and $-1 \le \upsilon \le 1$. It should be noted that the two ends of the Möbius strip are connected to each other after turning by angle π and therefore, the condition $\alpha(0,\upsilon) = \alpha(2\pi,-\upsilon)$ is valid where $\alpha = x, y, z$. As Eqs. (4) – (6) show, the structural characteristic of the Möbius strip depends on both the length (radius) and width of strip. It is expected that the structural characteristic and, therefore, the physical properties of the Möbius strip depend on the ratio of length / width [21, 29]. The variation of this ratio causes the variation in the curvature of the Möbius strip and, in consequence, it changes the strain induced in the Möbius strip. It also changes the bound length between the carbon atoms. In the present study, we consider the length of the Möbius strip to be constant and equal to 18 and the Möbius strip width varies from 2 to 6.

Table 1. *Effect of multiplicity on cohesive energy of graphene Möbius strip for different widths N=2, 3, 4, 5, 6. The minimum values of cohesive energy are shown by bold font.*

Cohesive Energy (eV/atom) / Multiplicity	N=2	N=3	N=4	N=5	N=6
2s+1=1 (Singlet)	-10.02	-10.01	-9.84	-9.52	-9.37
2s+1=3 (Triplet)	-10.28	-10.13	-10.09	-9.61	-9.52
2s+1=5 (Quintet)	-10.17	-10.30	-10.18	-9.78	-9.65
2s+1=7 (Septet)	-10.13	-10.23	-10.14	-9.92	-9.78

Now, we change the multiplicity (i.e., 2S+1 where S is the spin) of Möbius strip when its electric charge is maintained equal to zero and then we calculate the cohesive energy. The results are shown in table 1 for different widths of Möbius strip i.e., N = 2, 3, 4, 5, and 6. As the table shows, the cohesive energy is minimum when the multiplicity of Möbius is equal to 3 for N=2, is equal to 5 for N=3 and 4, and is equal to 7 for N=5 and 6. Therefore, the multiplicity depends on the width of the Möbius strip and it increases by increasing the width. As shown in table 1, for all values of width N, the minimum value of cohesive energy occurs when the multiplicity (2S+1) is greater than 3, which shows that the spin of Möbius strip i.e., S must be greater than zero. Thus, the Möbius strip has non-zero spin and its total magnetic moment is non-zero. As a result, the graphene Möbius strip is a ferromagnetic. This is due to this fact that the Möbius strip has only one edge topologically [12]. This effect is in contrast with zigzag graphene nanoribbon which is anti-ferromagnetic [7].

Table 2. *Comparison of cohesive energy of Möbius strip and graphene ribbon for different widths.*

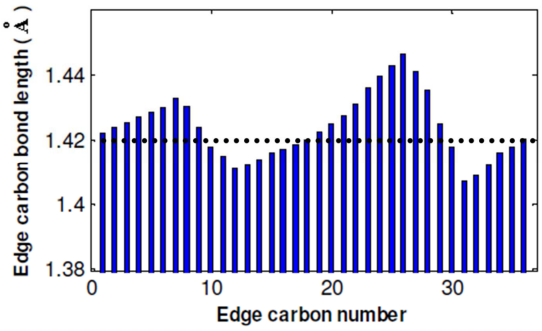
Cohesive Energy (eV/atom) / Structure	N=2	N=3	N=4	N=5	N=6
Möbius strip	-10.02	-10.01	-9.84	-9.52	-9.37
Graphene ribbon	-10.28	-10.13	-10.09	-9.61	-9.52

Table 3. *Comparison of band gap energy of Möbius strip and graphene ribbon for different widths.*

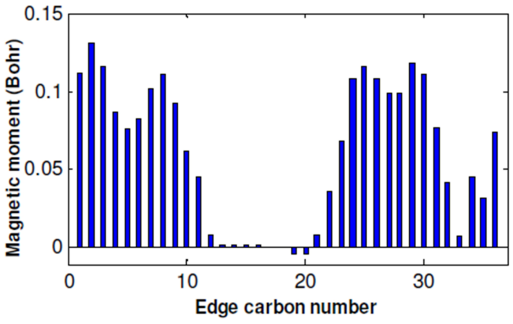
Band gap energy (eV) / Structure	N=2	N=3	N=4	N=5	N=6
Möbius strip	0.72	1.08	1.41	1.57	1.66
Graphene ribbon	0.67	0.89	1.09	1.21	1.13

In table 2, the cohesive energy of graphene Möbius strips is compared with that of graphene ribbons when the size (length and width) of graphene ribbons is chosen to be the same as the size of the Möbius strips. As table 2 shows, the cohesive energy of Möbius strips is greater than that of graphene ribbons. We know that the Möbius strips can be made by turning the graphene ribbons by angle π, and connecting two ends of ribbons to each other. In graphene ribbon the bound length between carbon atoms is equal to 1.42Å. The turning process causes the bound length of carbon atoms deviates from 1.42Å and induces strain in Möbius strips. In consequence, it is expected that the cohesive energy of Möbius strips increases relative to that of graphene ribbons with the same length and same width due to the deviation of bond length of carbon atoms or strain induced by turning process in the Möbius strips. Also, as we see in table 2, the cohesive energy depends on the width of the Möbius strip and it increases with increasing the width.

Now, we study the band gap energy of the Möbius strips. It is well known that the origin of band gap energy for graphene ribbons arises from the both quantum confinement and the crucial effect of the edges [30]. For graphene ribbons with zigzag edges, the gap appears because of a staggered sub-lattice potential on the hexagonal lattice due to the edge magnetization [30]. In zigzag graphene ribbon, when the width is less than 10Å, the band gap increases with increasing the width. The edge effect causes this increment [30]. When the width of ribbon is greater than 10Å the band gap energy decreases with increasing the width. This decrement is due to the confinement effect [30]. Table 3 shows the band gap energy of Möbius strip for different widths. For comparison, the band gap energy of graphene ribbon with the same width and length is also shown in this table. As the table shows, the band gap of Möbius strips is greater than that of graphene ribbons. Also, with increasing the width of Möbius strip, the band gap increases. This is due to the increment of the curvature of Möbius strip and, therefore, increment of strain.



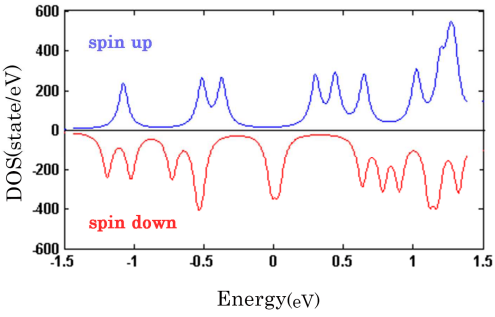
(a)



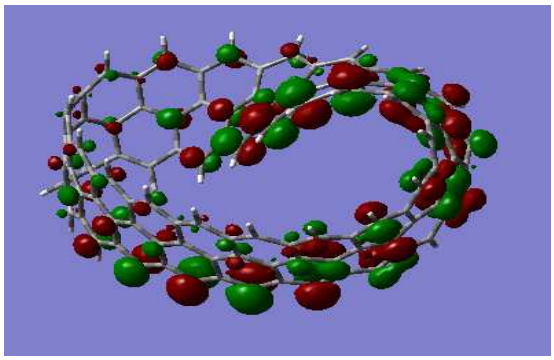
(b)

Fig 2. *(Color online) (a) Edge carbon bond length and (b) edge carbon magnetic moment as a function of the carbon atom number. Here, the length and width of graphene Möbius strip are L=18 and N=3. The dashed line in (a) shows the bond length of graphene sheet.*

Figure 2 shows the edge carbon bond length between the edge atoms and the magnetic moment as a function of the carbon atom number for Möbius strip with width N=3. The bond length can be defined as the average distance between a carbon atom and the first nearest neighbors. As Fig. 2(a) shows, the edge bond length between the atoms of Möbius strip depends on the position of edge atoms and it is greater than the graphene (sheet) bond length (i.e., 1.42 Å) for edge carbon numbers 1-9, 19-29. For other edge carbon numbers, the edge bond length of Möbius strip is less than the graphene bond length. The magnetic moment of each atom is defined as the multiplication of spin density of atom to the Bohr magnetization. As shown in Fig. 2(b), the magnetic moment of Möbius strip is non-zero which shows that the graphene Möbius strip made of zigzag graphene ribbon is ferromagnetic. This effect is in contrast with the zigzag graphene ribbons which are anti-ferromagnetic [7]. The variations of Möbius magnetic moment depends on its edge bond length and it reaches to its maximum values when the Möbius edge bond length reaches near the graphene sheet bond length (i.e., 1.42 Å) [see Figs. 2(a) and 2(b)]. In other words, the magnetic moment decreases with increasing the deviation of Möbius edge bond length from the graphene sheet bond length. Note that the deviation of edge bond length of graphene Möbius strip is due to its curvature and its strain. To calculate the magnetic moment we used Local Spin Density Approximation (LSDA) method i.e., we consider four vectors (ρ, m) where ρ is the density of electrons and, m is the magnetization vector [31].



(a)



(b)

Fig 3. *(Color online) (a) Spin-dependent density of states of Möbius strip as a function of the electron energy and (b) molecular orbitals of Möbius strip at E=0 eV.*

We now calculate the spin-dependent electronic density of states (DOS). Figure 3(a) shows the spin-dependent DOS of the Möbius strip versus the electron energy. For comparison between DOS of the spin up and spin down, the DOS of the later is shown with negative values. The Möbius strip length and width are the same as those in Figs. 1 and 2 (i.e., L=18 and N=3). As shown in Fig. 3(a), the value of DOS for spin up is not equal to that of spin down especially at E=0 eV which shows that the Möbius strip is a ferromagnetic. The non-zero DOS at E=0 in Möbius strip is due to the existence of surface (or edge) density of states. Figure 3(b) shows the molecular orbitals (MO) of electrons for Möbius strip at E=0 eV. It is seen that the orbitals are localized near the edge of Möbius strip which confirms the existence of edge states.

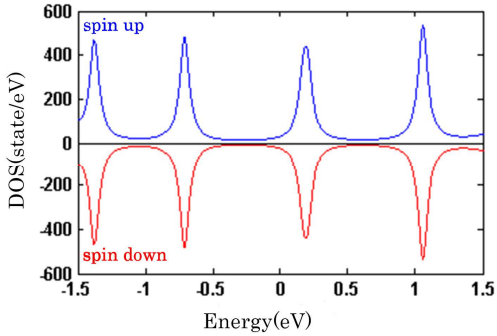
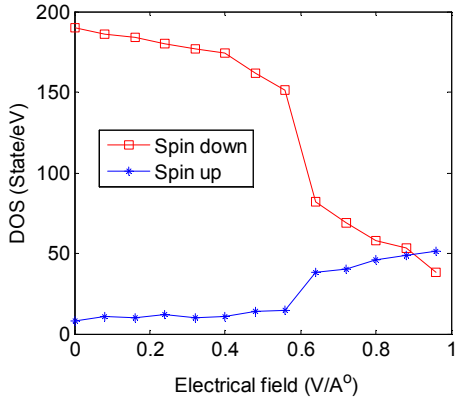


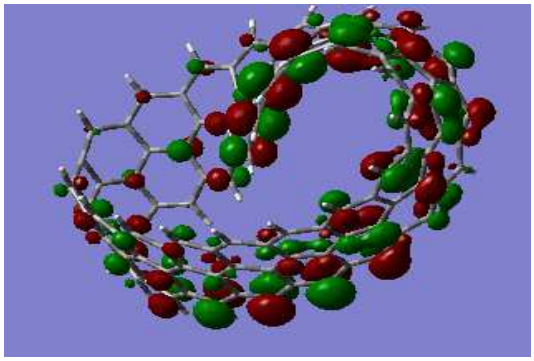
Fig 4*. (Color online) Spin-dependent density of states of a CNT with length L=18 and width N=3.*

As mentioned above, the graphene Möbius strip is made by turning a zigzag graphene nanoribbon (ZGNR) by angle π. To study the effect of this turning i.e., the topological effect on the DOS, a carbon nanotube (CNT) made of ZGNR with the length and width same as those of Möbius strip, is considered and its DOS is compared with the DOS of graphene Möbius strip. Figure 4 shows the spin dependent DOS of the above mentioned CNT. As shown in Fig. 4, the DOS of spin up and spin down electrons is equal for all values of electron energy which shows that the CNT is an antiferromagnetic. Comparing Fig. 4 with Fig. 3(a), it can be concluded that the ferromagnetic effect of Möbius

strip at E=0eV is due to the topological property of it.



(a)



(b)

Fig 5. *(Color online) (a) Spin-dependent density of states as a function of the external electric field at E=0 and (b) molecular orbitals of Möbius strip in the presence of applied electric field with strength 0.5V/Å.*

We now investigate the effect of an external electric field applied in the axis direction of Möbius strip (z-direction, see Fig. 1). Figure 5(a) shows the spin-dependent density of states at E=0 eV as a function of external electric field. As the figure shows, the density of states for spin up electrons increases with increasing the electric field, while for spin down electrons, the density of states decreases. There is a critical value for electric field [i.e., $E = E_{cr} = 0.84$V/ Å, see Fig. 5(b)] at which the density of states for spin up electrons becomes equal to that for spin down. When the electric field strength is greater than this critical value, the density of states for spin up electrons becomes larger than that for spin down. As a result, spin-flipping from down to up can take place when an electric field higher than the critical electric field is applied. As shown in Fig. 5(a), the density of states of both spin up and spin down at *E=0* is not zero when an external electric field is applied [see Fig. 5(a)]. Therefore, a gap is not induced by electric field and thus the graphene Möbius strip keeps its metallic surface states. It means that an external electric field, as a perturbation, cannot destroy the non-zero density of states of graphene Möbius strip. In addition, the molecular orbitals of electrons (at *E=0*) is shown in Fig 5(b) for Möbius strip in the presence of an external electric field. As we see in this figure, same as Fig. 3(b), the orbitals are localized near the edge of Möbius strip which confirms the existence of edge states even in the presence of a perturbation field.

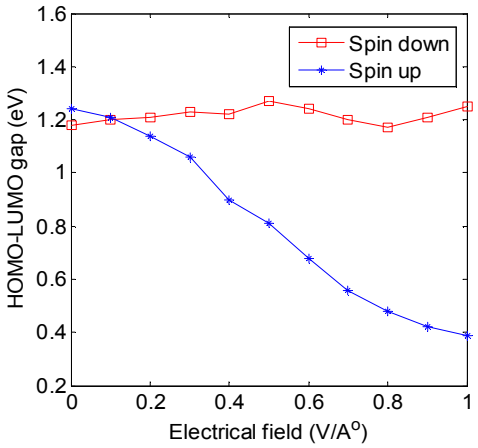


Fig 6*. (Color online) Spin-dependent HOMO-LUMO gap as a function of the external electric field.*

Figure 6 shows the spin dependence band gap energy of Möbius strip as a function of the external electric field. As shown in this figure, the band gap of spin down electrons is approximately remain constant, while the band gap of spin up electrons decreases by increasing the strength of electric field but it never becomes zero. It means that in spite of graphene nanoribbon which is a half-metal [8, 32], the Möbius strip can act as a half-semiconductor. Note that the term half-semiconducting is referred to the states having different α (spin-up) and β (spin-down) energy gaps [33].

4. Summary and Conclusion

The electronic and magnetic properties of graphene Möbius strips with different widths have been studied using DFT method. It has been shown that the multiplicity and cohesive energy of Möbius strip depend on the width of strip and they increase by increasing the width. Also, we have shown that the band gap of Möbius strip increases by increasing the strip width. Using local spin density approximation, the magnetic moment of Möbius strip is calculated and shown that the Möbius strip has ferromagnetic property and its magnetic moment decreases due to the strain induced by the curvature of Möbius strip. Under an external electric field applied in the axis direction of Möbius strip, the properties of Möbius strip have been studied and shown that the Möbius strip keeps its metallic surface states in the presence of an external electric field. Also, it has been shown that for electric field strength higher than a critical value, spin flipping from down to up can take place. In addition, the Möbius strip behaves as a half-semiconductor. The interesting properties of graphene Möbius strips that are different from graphene nanoribbons and nanotubes, such as ferromagnetism and spin flipping properties, may lead to interesting application of graphene Möbius strips in the electronic and spintronic devices.

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