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Electronic Band Structure and Magnetic Properties of Naked Zigzag Graphene Nano Ribbons Lying Symmetrically

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ABSTRACT

We have studied the electronic band structures and magnetic properties of the naked zigzag graphene nano ribbons lying symmetrically on the ribbon's middle under an external tensile strain along the edge direction by using first principle calculations. We have found that the ground state of unstrained line defects zigzag graphene nanoribbon's was antiferromagnetism in which the magnetic moment localized on the line defect was negligible. When an external tensile strain was applied along the edge direction, the energy band near the Fermi level is spin-split. The band splitting was enhanced with increasing the strain, leading to an increase of the local magnetic moments on the defect. Graphene nanoribbons with zigzag edges are characterized with special localized states, showing a ferromagnetic order in the same edge but antiferromagnetic order between two opposite edges. The ferromagenetic ordering has been found to exist in graphene materials with defect such as vacancies, topological defects, edges and hydrogen chemisorptions. When the defect position changes a transmission from an antiferromagnetism semiconductor to an antiferro magnetism half metal appears. The tensile strain along the zigzag direction of graphene with topological line defects. The antiferromagnetic coupling between the magnetic moments on the edges and the line defects leaded to a turnover of polarization direction on one edge of a critical value of the tensile strain, causing the line defect zigzag graphene nanoribbon to be ferromagnetic. The obtained results were found in good agreement with previous results.

KEYWORDS

Electronic band, zigzag graphene nanoribbon, tensile strain, line defect, antiferromagnetism, ferromagnetism, Fermilevel.

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INTRODUCTION

Graphene has been confirmed mechanically as a strong material which is able to sustain reversible elastic deformations in excess of 20% [1]. An applied strain is a useful way to tailor the graphene's electronic and magnetic properties [2-5]. A strain along the graphene's zigzag direction leaded to a gap opening at large deformations. Kou et al. [6] have shown that the tensile strain along the zigzag direction of graphene with topological line defects can greatly enhance the local magnetic moments on the line defects. A new type of topological line defect in graphene composed of octagonal and pentagonal sp^2- hybridized carbon rings has been

observed which was found to be a metallic wire [7]. The line defect divides a graphene sheet into two domains, both of which have the zigzag crystallographic directions along the line defect. It has been found theoretically that when the line defect was introduced into a zigzag graphene nano ribbon, the localized states on the line defect affected its magnetic behaviour. When the line defect position changes a transition from an antiferromagnetic semiconductor to an antiferromagnetic half metal appeared [8]. Graphene an important two dimensional carbon allotrope has been a hot topic due to its extraordinary mechanical, electronic [9], optical and magnetic [10] properties. Both the graphene and the quasi one dimensional graphene nanoribbons have been extensively studied in theoretical and experimental works [11-17]. The graphene nanoribbon's magnetism has attracted its promising applications in the design of nanoscale magnetic and spintronics devices [18-19]. Kumar et al. [20] made theoretical study of the electronic and magnetic properties of iron clusters encapsulated in carbon nanotubes using density functional theory. They have considered cluster encapsulated inside finite pieces of single wall zigzag nanotubes of indices (11,0) and (10,0). Finite zigzag nanotubes have a particular magnetic structure, the ground state is an antiferromagnetic spin singlet $s = 0$. The local spin polarization oscillates along the direction of the nanotubes axis and is small, except at the two ends of the edges of the nanotubes. They found that magnetism was confined within the iron aggregates with small reduction of the magnetic moment per atom with respect to the free iron clusters. Kumar, et al. [21] studied and calculated the diamagnetic coefficient for the neutral excitions confined in wobbled semiconductor self assembled quantum rings. They also studied symmetrically the impact of the rings reflection symmetry on the excitons ground state wave function localization, energy and diamagnetic coefficient. They have found that for the noninteracting particles, the electron wave function is staler to the unbalanced in the ring reflection symmetry than the whole wave function. The effective lateral radii of the electron and whole shrinking rapidly when absolute values of the parameters are growing. They have also found that a correction imbalance in the ring geometry and material content has a recognizable impact on the ground state energy of the neutral excitions.

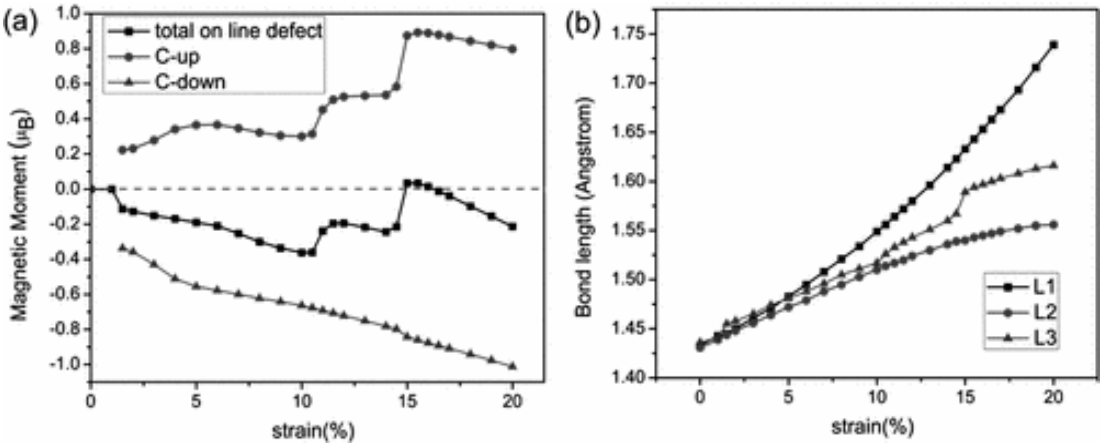
METHOD

The line defect in a unit cell of the line defect zigzag graphene nanoribbon was composed of one octagonal and a pair of pentagonal sp^2-hybridized carbon rings. A line defect separates a zigzag graphene nanoribbon into two parts with zigzag edges, which is denoted as the left and right ribbons. N_1 and N_2 are used to denote the zigzag edge with a line defect. N_1 and N_2 represent the numbers of zigzag chains in its left and right ribbons. We have used $N_1 = N_2$, because the positions of the line defect in the zigzag graphene nanoribbon has a big effect on its magnetic properties. Electronic and magnetic properties have been calculated using the spin polarized density functional theory in the generalized gradient approximation. The exchange correlations functional have been employed for the purpose of work. A large supercell along the width direction of the line defect zigzag graphene nanoribbons has been used to simulate isolated quasi one dimensional line defect zigzag graphene nanoribbon, making the closest distance between two adjacent line defect zigzag graphene nanoribbons 15 Å. The ribbon was placed along the Y- direction and large vacuum volume region was added in both *x* and *z* directions. A plane wave cut off of 520 eV was used in the simulations and energies were converged to 10^{-5} eV/atom. Both atomic positions and the lattice constant along the ribbon axis was fully relaxed unit, the maximum residual forces on atoms were less than 0.005 eV/Å. The obtained results were compared with previously obtained results.

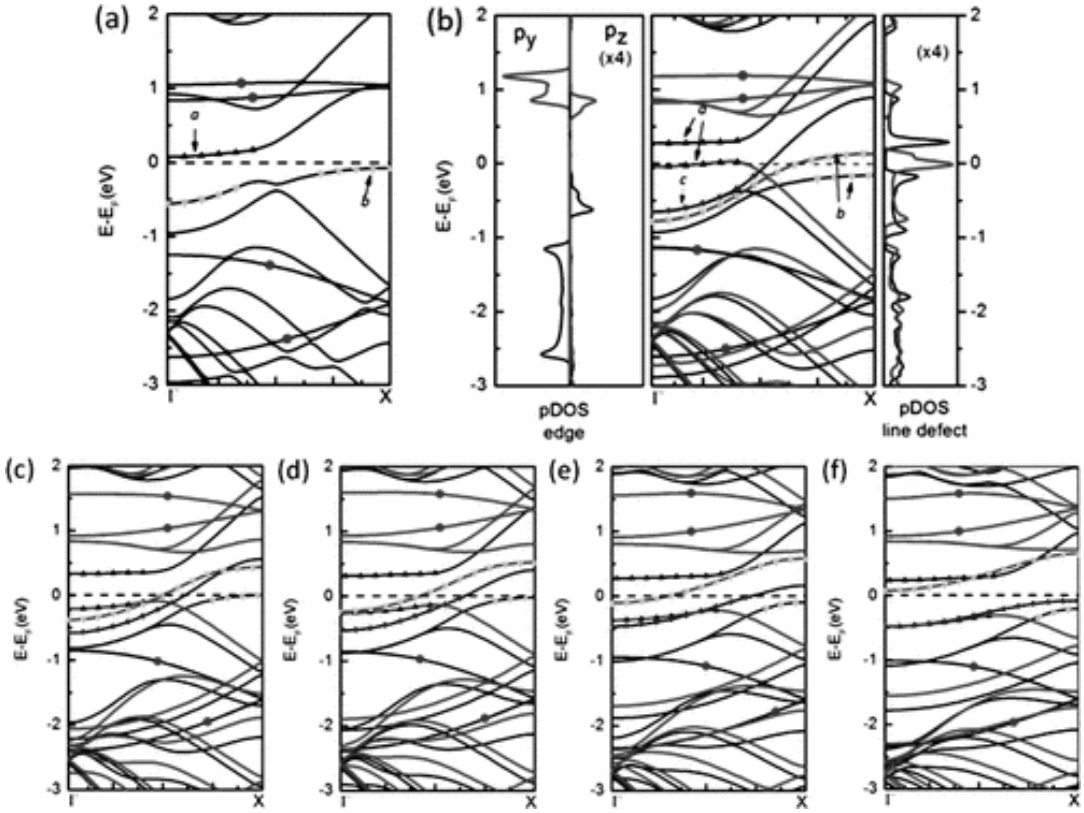
RESULTS AND DISCUSSION

Graph (1) shows band structures of line defect zigzag graphene nano ribbon under different stains where the spin-up and spin down bands are shown without strain is in the anntiferromagnetism state in which the spin-up and spin down bands are degenerate with an indirect band gap of about 0.15eV. There are two flat bands near the Fermilevel, labeled as a and b which are marked by triangles inverted triangles as shown in graph (2). As the strain increases flat bands near the Fermilevel become spin split. We have calculated densities of states of the system at different strains in the ferromagnetic state for p orbitals of the edge atoms and p_z orbital of the carbon atoms on the line defect which have been shown on the left and right sides of the band structure as shown in graph 2(b). There is a spin-up band crossing the Fermilevel with its occupied part contributed mainly by the p_z orbitals of the edge atoms, which is labeled as C and marked as dot in graph 2(b) to 2(f). With the increase of external strain, the spin splitting was enhanced gradually. We have found that the spin down a band descends and the spin down b band ascends while the spin up b band first rised as the strain varied and then fallen. When the strain further increased, leading to the oscillating behaviour of magnetic moment on the line defect. The spin-up c band gradually descends as the strain increase, indicating an increase of the orbital occupation of edge atom, which leaded to the increase of magnetic moments of the edges. Graph (3) shows the depenedence of total magnetic moment and the ferromagnetic state stability on the ribbon's width. The obtained results showed that the energy difference ΔE is always negative indicating that the ferromagnetic configuration is more stable than

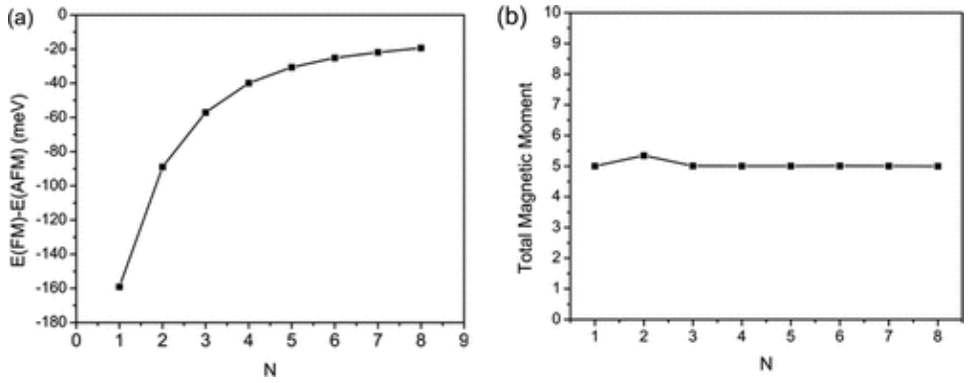
the antiferromagnetism one when the width increased forn N=1 to 8. The absolute value of ΔE decreases as the width increases and might eventually vanish at a very large ribbon width. The The obtained results were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.



Graph 1: The total magnetic moment on its line defect and the corresponding local magnetic moments on the C-up (i.e. C2, C3, C4-type) and C-down (C1-type) carbon atoms versus the external strain. (b) The bond length variation of three key bonds versus the external strain.



Graph 2: The spin polarized band structures of 3-3- LD-ZGNR in a unit cell under different strains.



Graph 3: (a) The energy difference $\Delta E = E_{FM} - E_{AFM}$ per unit cell between its FM and AFM configuration varies with ribbon's width

CONCLUSION

The electronic band structure and magnetic properties of naked zigazag graphene nanoribbon have been studied theoretically applying external tensile strains. We have found that the applied strain induced the local magnetic moments on the line defect, whose coupling with those on the edges leaded to a turnover of the spin polarization on one edge making the line defect zigzag graphene nanoribbon became a ferromagnetic metal at a large enough strain. Calculated total magnetic moment per unit cell as a function of ribbon;s width indicated that its value remained almost unchanged at a value of about $5\mu_B$ as the width increased. The band splitting was enhanced with increasing the strain leading to an increase of the local magnetic moments of the line defect. The obtained results suggested a possible way to tune the magnetic and transport properties of zigzag graphene nanoribbon by applying strain. The obtained results were found in good agreement with previously obtained results.

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