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Effects of vertical strain on zigzag graphene nanoribbon with a topological line defect

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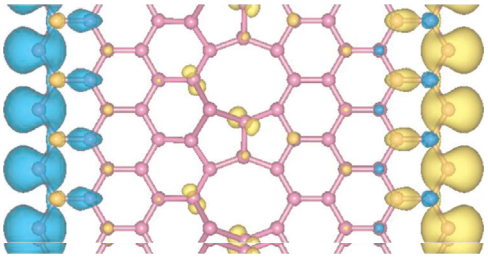
HIGHLIGHTS

- For a given deformation size, the strain energy increases with increasing vertical distance.
- For a fixed vertical distance, a smaller deformation zone generates larger strain energy.
- A local spin distribution appears in the deformation region.

GRAPHICAL ABSTRACT

The elastic, electronic and magnetic properties of the zigzag graphene nanoribbon with a topological line defect are investigated under vertical strains using first-principles calculations.



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ABSTRACT

We report the elastic, electronic and magnetic properties of naked ZGNRs with topological line defects (LD-ZGNRs) lying symmetrically on the ribbon's middle under vertical strains at four types of line defect atoms by using a first-principles approach. By changing the position and size of the local deformation of the ribbon, the optimal position is obtained. Moreover, an apparent spin-splitting of the energy band is obtained when a local deformation is created by the vertically applied strain.

1. Introduction

Since its first appearance in 2004 [1], graphene has attracted tremendous interest because of its unique linear energy band near the Fermi energy and concomitant novel physical and chemical properties [2,3]. Graphene nanoribbons (GNRs) are nanometer-sized stripes of graphene sheets, and have been prepared experimentally by cutting mechanically exfoliated graphenes [1,4–6] or chemical means [7,8]. The electronic and magnetic properties of GNRs have been widely studied [9–11]. Both first-principles computations [12] and experimental investigations [13] have revealed a nonzero band gap for GNRs independent of their width and chirality. According to the edge termination types, the GNRs are generally classified into two basic groups, i.e., the armchair and zigzag GNRs (AGNRs and ZGNRs) [6,12–14]. It is now well-known that ZGNRs have shown magnetism by theories due to the localized edge states [10,11] which opens up possibilities of making graphene-based low-dimensional magnetic nanostructures [15] and potential applications of ZGNRs in spintronics [11,16].

Theoretically, various methods such as carrier injection, oxidation of two sides, application of a magnetic field in the substrate,

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application of an in-plane electric field, doping, hydrogenation or fluorination at the edges have been proposed to tune the magnetic and electronic properties of the ZGNRs [17–20]. Moreover, a study of defects in this material is critically important. In particular, a new type of one-dimensional topological line defects (LD) in graphene has recently been produced experimentally. This new line defect structure is found to be a metallic wire and may play important roles in device application. Lahiri et al. have synthesized an extended line defect with two pentagon rings and one octagon ring (represented as the 5–8–5 defect for further discussion) in graphene by introducing a structural mismatch during its formation on the Ni(111) surface and shown that it had metallic nature [21]. In addition, it has been shown that for ZGNRs, the presence of the special types of topological line defect in one unit cell can alter the across-edge coupling nature from antiferromagnetic (AFM; which is the coupling nature of pure ZGNRs) to ferromagnetic (FM) resulting in a finite magnetic moment in the system [22,23].

Strains are also expected around defects in graphene [24], and their role should be considered wherever defects are involved, for instance when engineering electronic [25] or magnetic [26] properties using plasma etching or irradiation. Besides, many researchers apply vertical strain to graphene sheets to study their mechanical or electronic properties [27,28]. With this idea, we, in this work, investigate the ZGNR with a topological line defect at its middle (LD-ZGNR), parallel to its edges, and suffering vertical strain at line defect atoms by using first-principles calculations. We find that the position and size are both major factors to get favorable structure of the LD-ZGNR under vertical strain. Furthermore, the vertical strain could induce the local magnetic moments on the line defect. According to the numerical results, it is a good way to tune the elastic and magnetic properties of the LD-ZGNR by applying vertical strain, which is very useful for applications of the graphene ribbon in spintronics and electromechanical devices.

2. Computational methods

We have simulated LD-ZGNR in Fig. 1a, which is still a quasi-one-dimensional (Q1D) periodic system along its axis direction even though it has a line defect. A local vertical deformation is simulated by setting one carbon atom as the center of the circular deformation zone, and then pushing down the central atom vertically and fixing it at a certain distance d from the ribbon plane, as shown in Fig. 1b. We can examine the local magnetic moments on four types of line defect atoms, C1, C2, C3, and C4 separately. It is known from Fig. 1a that the line defect in a unit cell of the LD-ZGNR is composed of one octagonal and a pair of pentagonal sp^2-hybridized carbon rings. And a line defect separates a ZGNR into two parts, which can be represented as the left and right ribbons. Therefore, we can use a symbol of $N1$-$N2$-LD-ZGNR to mark the zigzag edge GNRs with a line defect, where $N1$ and $N2$ represent the numbers of zigzag chains in its left and right ribbons, respectively. For the sake of simplicity, we only study in this paper a simple case of $N1=N2=N$ because the position of the line defect in the ZGNR has a big effect on its magnetic properties [22].

Density functional theory (DFT) calculations [29,30] are carried out using first-principles plane-wave pseudopotential method through the Vienna ab initio simulation package (VASP) code [29–31]. The ion–electron interactions are treated with the projector-augmented plane wave (PAW) approach [32], and the exchange–correlation interactions were expressed with a generalized gradient approximation (GGA) in the form of the Perdew–Burke–Ernzerhof (PBE) functional [33]. A plane-wave cutoff of 500 eV is used in our simulations. The energies and the forces on each ion are converged within 10^{-4} eV and 0.02 eV/Å,

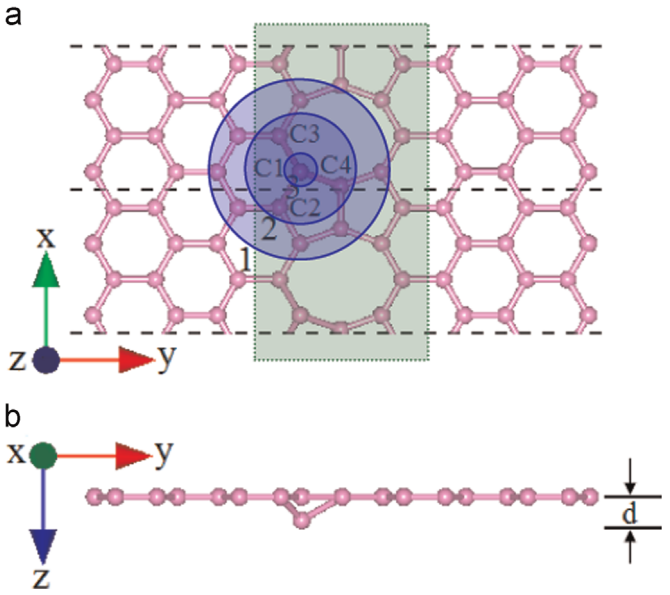

Fig. 1. (a) Top view structure of the pristine of a 3-3-LD-ZGNR, where the insides of green parallelograms denote the carbon atoms on the line defect. The line defect in each unit cell has 10 carbon atoms, which are divided into four types, C1, C2, C3, C4, based upon the structure symmetry. The central atoms and three deformation zones are marked as C1–C4 and blue circles 1–3, respectively. (b) Side view of the 3-3-LD-ZGNR under vertical strain, setting C1 as the central atom of the deformation zone as an example. All carbon atoms are magenta balls. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

respectively. The periodic boundary condition is set with the vacuum region between two neighboring nanoribbons larger than 20 Å and Brillouin zone integration is carried out using a $32 \times 1 \times 1$ Monchorst-Pack k-grid. The 2s and 2p orbitals of the carbon atom are treated as valence ones. A large supercell along the width direction of the LD-ZGNR is used to simulate the isolated Q1D LD-ZGNR. The ribbon is placed along the x direction, and large vacuum volume region is added in both y and z directions.

3. Results and discussions

3.1. Intrinsic strengths

Our DFT calculations have identified how the deformation of 3-3-LD-ZGNR has an impact on its elastic properties and intrinsic strength (defined as the stress point beyond which the stress decreases with strain). The effective force of 3-3-LD-ZGNR can be expressed as

$$F = \Delta E/\Delta d \quad (1)$$

with the vertical distance d (Fig. 1b), where ΔE means the total energy difference for two successive distances. As example, we choose the size of the deformation zone within the circle 2 indicated in Fig. 1a, the effective force versus deformation distance d is shown in Fig. 2, in which the curves C1, C2, C3, C4 mean deformations for four types of line defect with carbon atoms C1, C2, C3, C4 as their central atom, respectively. It is determined that the force increases with the increasing vertical distance d, meaning that a larger force is needed to produce deeper vertical deformation in the 3-3-LD-ZGNR. Interestingly, when the vertical distance is less than about 1.2 Å, curves C1 and C2 are nearly coincident with curves C3 and C4, respectively, which means that the environments of C1 and C3 are dramatically different from those of C2 and C4. The force decreases as the vertical distance is