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The electronic and magnetic properties of corrugated zigzag graphene nanoribbons with divacancy defects

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ABSTRACT

We investigate the electronic and magnetic properties of the corrugated zigzag graphene nanoribbons (ZGNRs) with divacancy defects by means of the first principle calculations. We show that the magnitude of corrugation in the defective ZGNR determines whether the system is in the antiferromagnetic state, in the ferromagnetic state, or in the nonmagnetic state. Correspondingly, the mutual transition between the semiconductor and the metal can also be realized in this structure. Moreover, for semiconductors the energy gap displays oscillating behaviors as the magnitude of corrugation increases. These results are identified as being useful in manufacturing flexible devices.

1. Introduction

Graphene, a two-dimensional network of carbon atoms, has attracted extensive interest due to its unique physical properties and promising applications in future nanodevices [1]. However, pure graphene is a zero gap semiconductor, which seriously hinders its way to use for logic electronics, thus raising the question of how to effectively tune the energy gap. One of brilliant strategies is to tailor the graphene sheet into zigzag nanoribbons (ZGNRs), which not only modifies the electronic structure but also brings the edge magnetism [2–4]. Such edge magnetism was shown to be very promising for applications in spintronics devices [5–8]. Besides processing the graphene sheet into nanoribbons, chemical doping [9–12], defects [13–15], and mechanical deformations such as strained [16–18], twisted [19], wiggled [20], folded [21], bended [22–24] structures, and graphene corrugations [25], also have significant effects on the electronic and magnetic properties of graphene. Corrugations inhere in the suspended graphene sheet [26], and can also be induced by substrates [27], defects [28], or adsorbates [29]. Such corrugations would lead to a long-range scattering potential in single-layer graphene, and severely modify the charge-carrier mobility [30] as well as spin-orbit couplings and spin relaxation [31]. In graphene nanoribbons (GNRs) [32–35], these corrugations also play a significant role in their electronic band structures [33,34] and transport properties [35]. Thus, understanding of how corrugations modify the electronic and magnetic properties of graphene and GNRs is a very important issue for the basic research.

From the practical standpoint, such knowledge is also very important for graphene's applications in flexible electronics [36], because the corrugations are difficult to avoid. On the one hand, in the process of fabricating graphene-based flexible devices, graphene is always put on a substrate, which may enhance the corrugations in graphene due to the interaction and the lattice mismatch between graphene and substrate surface. On the other hand, mechanical deformations or other factors can also cause graphene corrugations. Recently, numerous graphene-based flexible devices have been widely studied including energy conversion and storage [37–39], transistors [40,41], sensors [42,43], and wearable devices [44,45]. However, the role of corrugations is less considered.

In this paper we study the influences of corrugations on the electronic and magnetic properties of the ZGNR with divacancy defects. These defects might be created in regions of different curvature by

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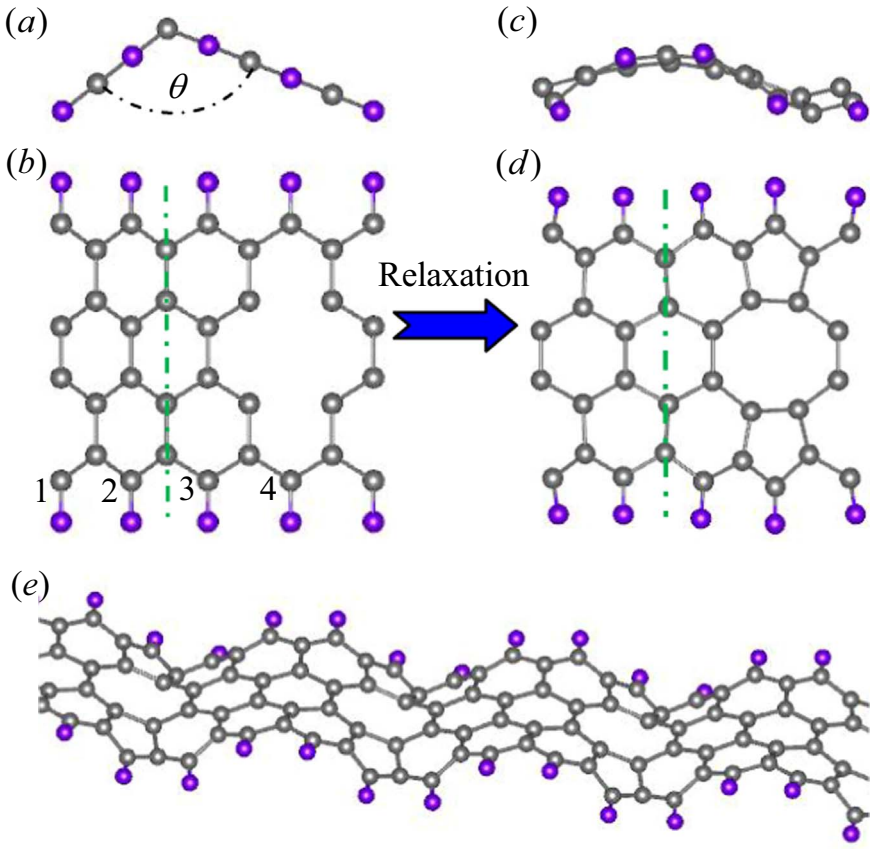

Fig. 1. (a) Side view and (b) top view of original model structural of DV-ZGNR in the periodic supercell. θ is the curvature angle before structure relaxation. (c) Side view and (d) top view of the model structural of DV-ZGNR after full relaxation. (e) Full view of optimized model structure for $\theta = 120^{o}$. The gray and the purple balls represent carbon and hydrogen atoms, respectively. The green line indicates the curved site. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

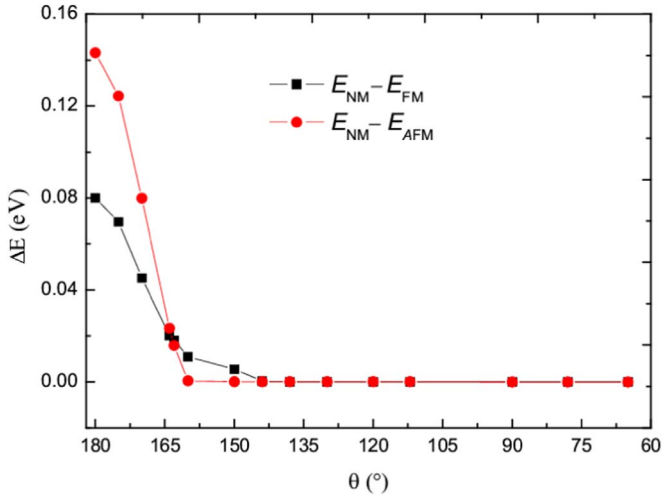

Fig. 2. The energy difference per supercell between the NM and the FM (AFM) state as a function of the curvature angle θ.

using a focused electron beam [46]. As we all know, vacancies can induce magnetic moment [47,48], and modify the electronic and phonon properties of graphene [49]. Moreover, the magnetism of vacancies in corrugated graphene can be controlled by altering the magnitude of corrugation under isotropic strain [50]. In the present work, we mainly focus on the role of the magnitude of corrugation. We will show that when the magnitude of corrugation increases the electronic property of ZGNR with divacancy defects experiences a semiconductor-metal-semiconductor transition, while for the magnetic property the system exhibits an antiferromagnetic-ferromagnetic-nonmagnetic phase transition. We further show that the energy gap displays oscillating behaviors when the system is tuned to the nonmagnetic state.

2. Model and method

The original structure was constructed by asymmetrically bending the ZGNR with double-vacancy defects in the periodic supercell. For convenience, this ribbon is denoted by DV-ZGNR. The degree of initial curvature is characterized by angle θ [see Fig. 1(a)], which determines the magnitude of corrugation when the curved site is fixed [see the green dashed line in Fig. 1(b)]. The double-vacancy locates in the vicinity of the border region of the supercell, and all the edge carbon atoms are saturated by hydrogen atoms to avoid dangling bonds.

Our calculations were performed in the framework of the spin-polarized density functional theory (DFT), as implemented in the plane-wave-basis-set VASP code [51]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) form [52] was employed to describe the exchange-correlation term. The core electrons were treated with projector augmented wave (PAW) potentials [53]. The plane wave cutoff energy was set to 500 eV, and further increasing this value had little effect on the results. The structures were relaxed until the energy and force on each atom were less than 10^{-6} eV and