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Structural and electronic properties of armchair graphene nanoribbons under uniaxial strain



Li-Hua Qu^a, Jian-Min Zhang^{a,*}, Ke-Wei Xu^b, Vincent Ji^c

^a College of Physics and Information Technology, Shaanxi Normal University, Xian 710062, Shaanxi, PR China

^b College of Physics and Mechanical and Electronic Engineering, Xian University of Arts and Science, Xian 710065, Shaanxi, PR China

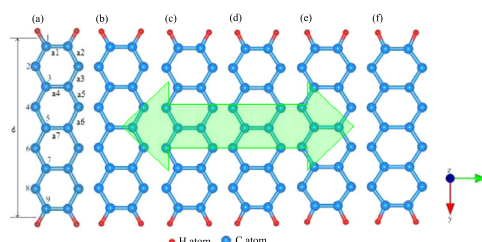
^c ICMMO/LEMHE, Université Paris-Sud 11, 91405 Orsay Cedex, France

HIGHLIGHTS

- Each bond length decreases (increases) with increasing compression (tension) strain.
- At a certain strain, the average energy increases with decreasing the ribbon width n .
- Average energy increases quadratically with the absolute value of the uniaxial strain.
- Dependence of the band gap on the strain is sensitive to the three ribbon width families.
- Each ribbon width family leads to oscillatory band gaps due to quantum confinement effect.

GRAPHICAL ABSTRACT

From (a) $\epsilon = -6\%$ to (f) $\epsilon = 9\%$, although the length of the bonds a1 to a7 increases, the ribbon geometrical width d decreases.



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ABSTRACT

We theoretically investigate the structures, relative stabilities and electronic properties of the armchair graphene nanoribbons (AGNRs) under uniaxial strain via first-principles calculations. The results show that, although each bond length decreases (increases) with increasing compression (tension) strain especially for the axial bonds a1, a4 and a7, the ribbon geometrical width d increases (decreases) with increasing compression (tension) strain due to the rotation of the zigzag bonds a2, a3, a5 and a6. For each nanoribbon, as expected, the lowest average energy corresponds to the unstrained state and the larger contract (elongate) deformation corresponds to the higher average energy. At a certain strain, the average energy increases with decreasing the ribbon width n . The average energy increases quadratically with the absolute value of the uniaxial strain, showing an elastic behavior. The dependence of the band gap on the strain is sensitive to the ribbon width n which can be classified into three distinct families $n=3l$, $3l+1$ and $3l+2$, where l is an integer. The ribbon width leads to oscillatory band gaps due to quantum confinement effect.

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1. Introduction

Graphene nanoribbons (GNRs) have been studied experimentally and theoretically, especially for their unique electronic

structures [1–3] and transport properties [4–6] due to the quasi-one-dimensional nature [7] and the formation of a band gap, which will lead to potential applications in both optoelectronic and nanoelectronics [8–11]. The electronic structures for GNRs can be modified by doping, disorder [12,13] and external fields [14]. Recently, people have paid much attention to the mechanical strain influence on graphene systems since the naturally or intentionally tensional strain may be inevitable in graphene-based electronic

* Corresponding author. Tel.: +86 2985308456.

E-mail address: jianm_zhang@yahoo.com (J.-M. Zhang).

devices [14,15]. Strain arises when a crystal is compressed or stretched out of equilibrium, with the stiffness tensor providing the constitutive relation between applied stress and final strain state. Atomic relaxations often accompany the process, also resulting in an effective renormalization of the constitutive relations.

Theoretically, the first-principles [16] and tight-binding calculations [17,18] on the electronic structure for a suspended graphene under uniaxial strain have been studied. These studies revealed that the presence of strain can significantly affect the device performance. The uniaxial strain can be induced by bending the substrates on which graphene is elongated without slippage [19–21]. Elastic responses have been measured by pushing a tip of atomic force microscope suspended graphene [22,23,24]. Nevertheless, it is still not clear what the combined effects of the strain are, on the band gap of armchair graphene nanoribbons (AGNRs).

Herein, we performed detailed first-principles computations to reveal the atomic and band structures of the AGNRs under uniaxial strain. The following questions are mainly addressed: (1) What would these structures look like if an uniaxial strain is applied on these AGNRs? (2) Do the fully hydrogenated AGNRs have favorable formation energies under uniaxial strain, and how about their size effects? (3) Is there any related phenomena corresponding to the electronic structures? The answers to these questions will give us a deeper understanding of the atomic and band structures of strained AGNRs, and a guide for better usage of these materials in future graphene-based functional nanodevices. In the light of these density functional theory (DFT) computations [25], we can modulate the band gap of AGNR effectively through uniaxial strain. Thus it is highly feasible that these intriguing properties can be fabricated in the AGNR-based nanomaterials, which is advantageous for the design of automatic integration.

2. Method and model

All calculations were performed by using the Vienna *ab initio* simulation package (VASP) code [26–28]. The projected augmented wave (PAW) [29] pseudopotentials are employed and the exchange-correlation energy is treated with the local density approximation (LDA) adopted with a 450 eV cutoff energy. Reciprocal space was sampled by $40 \times 1 \times 1$ using Monkhorst Pack meshes centered at the Γ point. 20 K-points were included in band

structure calculations along Γ (0, 0, 0) to X (0.5, 0, 0). The total energies are converged to 10^{-4} eV and atoms are fully relaxed until the magnitudes of the forces less than 0.1 eV/nm. The vacuum distance between two adjacent ribbons is 20 Å (*y* and *z* directions) to eliminate interaction due to periodic boundary condition.

In our calculations, the AGNRs are classified by the armchair chains across the ribbon as shown in Fig. 1(a) for 9-AGNR. The uniaxial strain is imposed by increasing the lattice constant of the AGNR in the *x*-direction, and strain (ϵ) is defined as [30]

$$\epsilon = (L - L_0)/L_0 \quad (1)$$

where L and L_0 are the deformed (stretched or shrunken) and initial equilibrium lattice constants ($L_0 = 4.26$ Å).

3. Results and discussions

3.1. Geometric structures and relative stability

As examples, the optimized geometrical structures of 9-AGNR terminated with H atoms are shown in Fig. 1, where the strains for the structures (a), (b), (c), (d), (e) and (f) are -6% , -3% , 0% , 3% , 6% and 9% , respectively. The optimized bond lengths of the seven C–C bonds as labeled by a1, a2, a3, a4, a5, a6 and a7 in Fig. 1(a) and the ribbon geometrical width d in the *y*-direction are listed in Table 1 for 9-AGNR under different uniaxial strains. As can be seen in Fig. 2, firstly, at each strain, the edged axial bond a1 is the shortest among the seven C–C bonds. Second, although each bond length decreases (increases) with increasing compression (tension) strain

Table 1

The optimized lengths of the seven C–C bonds a1, a2, a3, a4, a5, a6 and a7 and the ribbon geometrical width d in the *y*-direction for 9-AGNR under different uniaxial strains along the periodic direction *x*.

Strain (%)	a1 (Å)	a2 (Å)	a3 (Å)	a4 (Å)	a5 (Å)	a6 (Å)	a7 (Å)	d (Å)
−6	1.33	1.39	1.39	1.36	1.40	1.40	1.36	11.74
−3	1.35	1.39	1.40	1.39	1.41	1.40	1.39	11.71
0	1.36	1.40	1.41	1.42	1.42	1.41	1.43	11.67
3	1.38	1.41	1.42	1.46	1.43	1.42	1.47	11.64
6	1.39	1.42	1.43	1.50	1.44	1.44	1.51	11.57
9	1.41	1.43	1.44	1.55	1.45	1.43	1.56	11.56

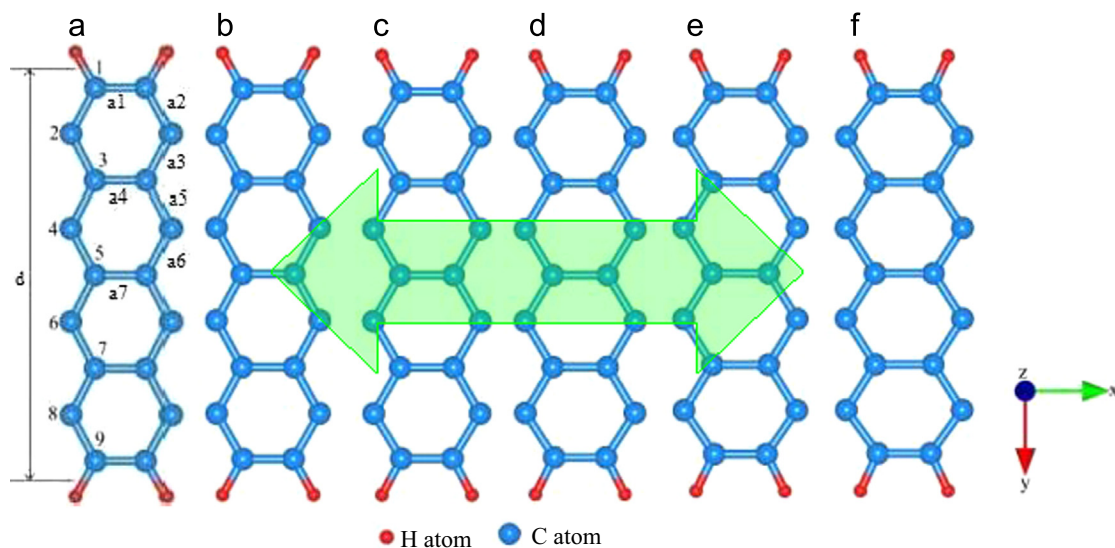


Fig. 1. Optimized structures of 9-AGNR drawn by uniaxial strains: (a) $\epsilon = -6\%$; (b) $\epsilon = -3\%$; (c) $\epsilon = 0\%$; (d) $\epsilon = 3\%$; (e) $\epsilon = 6\%$ and (f) $\epsilon = 9\%$ along the *x*-direction. The axial bonds a1, a4 and a7 and the zigzag bonds a2, a3, a5 and a6 are indicated in panel (a) together with the ribbon geometrical width d .

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