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Effects of Stone-Wales Defect Symmetry on the Electronic Structure and Transport Properties of Narrow Armchair Graphene Nanoribbon

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ABSTRACT

We report a first principles calculation to investigate the electron transport properties of defected armchair graphene nanoribbon (AGNR) influenced by Stone-Wales (SW) defect. The SW defect is found to be able to effectively influence the electronic structure of the defected AGNRs, and their electron transport behaviors can exhibit prominent differences depending on the symmetry of the nanostructured morphology. Moreover, our simulations have revealed that the introducing of the SW defect could be favorable for the electron transport of the defective AGNR. Our investigation has confirmed the possibility of tuning the electron transport of graphene nanoribbon by introducing a topological defect, which could be helpful to extending the field of applications for graphene nanoribbon-based nanodevices.

1. Introduction

Graphene, a truly two dimensional (2D) nanomaterial arising from a hexagonal carbon lattice in a single layer, has been widely regarded as the most promising candidate for the application of the next generation of nanodevices since its fabrication in 2004 [1]. However, a major impediment for the practical applications of graphene has been the absence of a band gap in this nanomaterial [2]. Many experimental studies have been devoted to engineering a band gap for graphene nanomaterials [3] and various fabrication strategies have been proposed [4], mainly including epitaxial growth, substitutional doping, quantum confinement, and chemical functionalization. The quasi-one-dimensional graphene nanoribbons (GNRs) are an important component because a significant band gap can be experimentally realized in narrow GNRs in terms of quantum confinement at room-temperature [5], which facilitate high switching ratios in GNR-based transistors [6]. More importantly, a broad range of applications for GNR-based nanodevices are expected to be tested in the near future because large-scale GNR fabrication has been successfully demonstrated by using patterning and etching routes [7] as well as a longitudinal unzipping carbon nanotube route [8].

Considerable amounts of studies relevant to GNRs have been carried out for the fundamental understanding of their electronic structure [9], electron transport [10], optical [11,12], and mechanical [13] properties, as well as atomic reconstruction in GNRs [14–16]. It is found that the formation of the GNR edges has essentially influenced their electronic and transport properties [17]. The armchair and zigzag GNRs, according to the atomic arrangement pattern of their edges [9], have recently attracted extensive attention [18,19]. In particular, a great effort has been focused on controllable manipulation of electronic and transport properties of armchair and zigzag GNRs in a useful range [20], which are of vital importance to achieving GNR-based nanodevices [4]. Both theoretical calculations [19] and experimental studies [21] have shown that the electronic transport properties of GNRs can be dramatically altered by introducing disorder, such as vacancies [22], topological defects [23], adsorption [24], substitutional doping [25], adatom [26], and chemical functionalization [27]. Meanwhile, experimental measurements on GNRs can provide global information of not only their atomically resolved nanostructure but also their electronic states by using characterization techniques [2], such as transmission electron microscopy (TEM), scanning tunneling microscopy (STM), and scanning tunneling spectroscopy (STS).

In the experimental research approach, energetic particle irradiation implemented in aberration-corrected high resolution TEM has offered an opportunity of precise modification of atomic structure of nanomaterials by introducing point defects [28], such as vacancies, adatoms, impurities, Stone-Wales (SW) defect, etc. More specifically, the SW defect, created by rotating a C–C bond by

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90° with respect to the midpoint of the bond, not only has the lowest transformation energy among all intrinsic defects in graphenic systems, but also is shown to be energetically more favorable than in carbon nanotubes (CNTs) or fullerenes [29,30]. Hence, point defects in carbon nanostructures inevitably accompanying the GNR fabrication strongly affect the electronic transport of this novel nanomaterial [31]. For instance, the presence of the SW defects is found to significantly enhance the anisotropy of spin-dependent transport properties of the ZGNRs [32]. Meanwhile, previous studies have shown that armchair graphene nanoribbons (AGNRs) are energetically more stable than zigzag graphene nanoribbons (ZGNRs) and thus the former have been more frequently characterized in experimental observations [33,34]. It has been demonstrated that the SW defects observed in the graphene nanomaterial can be introduced by energetic particle impacts, and such defects have high stability at room temperature once they are formed [35]. Consequently, a deep understanding of SW defect influences on the electronic transport of AGNRs is of great importance to the performance, design, and practical applications of GNR-based nanodevices.

In this article, we have reported the first principles calculation on the narrow AGNR consisting of symmetric and asymmetric SW defects to assess the influences of the defects on the electronic structure and transport properties of an AGNR nanomaterial. It is found that the introducing of the symmetric and asymmetric SW in narrow AGNR has distinct effects on the electron transport. The asymmetric SW defect is predicted to be favorable for the electronic transport properties, in contrast to the substantially decreased in the symmetric defected nanostructure. Our calculation results may be helpful to the development of GNR-based nanoelectronics.

2. Model and computational method

The atomically resolved AGNR reconstruction has been performed by using the density functional theory (DFT) utilized in the framework of the SIESTA code [36,37]. The Troullier-Martins pseudopotential has been chosen to deal with the interaction between the valence electrons and the atomic core [38]. We make

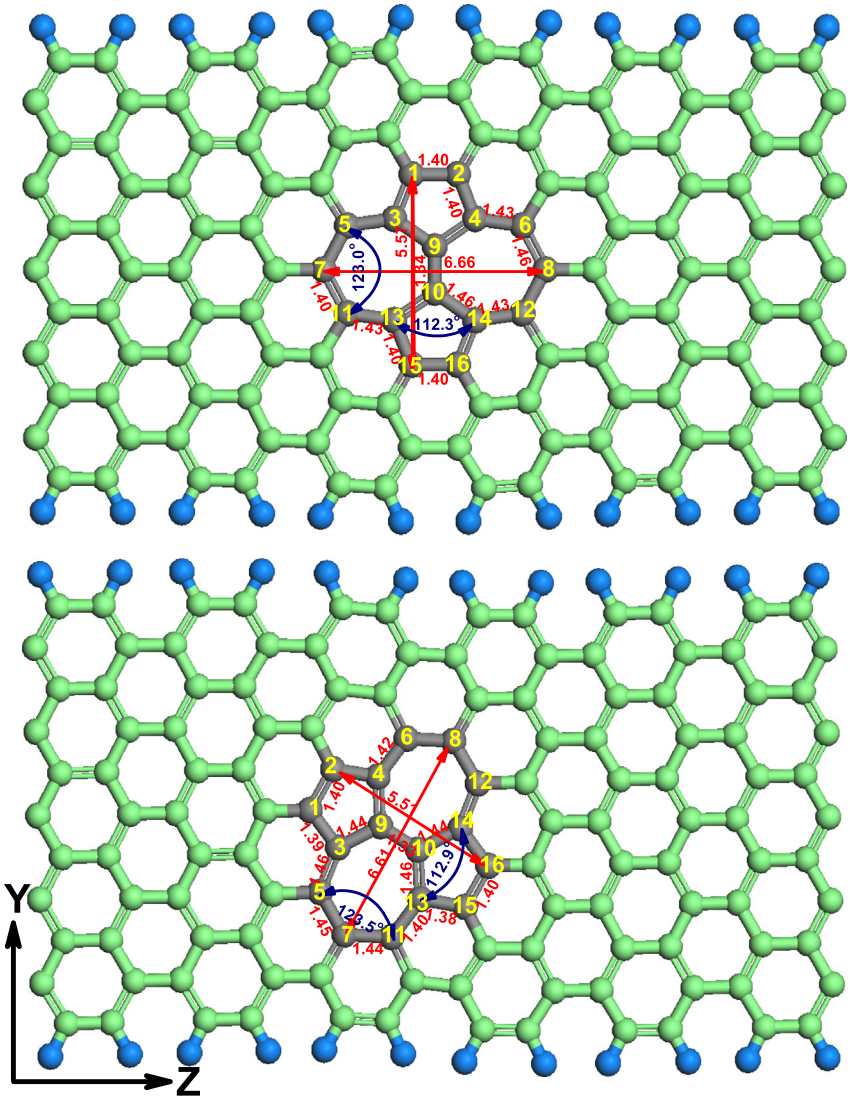

Fig. 1. Schematics of the reconstructed AGNR nanostructures in the presence of (a) the symmetric SW defect and (b) the asymmetric SW defect. The green colored atoms and blue colored atoms represent carbon and hydrogen atoms, respectively. The SW defects in nanostructure are highlighted by gray atoms. The C–C bond lengths (in Å) and angles (in degree) are depicted by the red numeral and blue numeral, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)