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The structures and electronic properties of zigzag silicene nanoribbons with periodically embedded with four- and eight-membered rings

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ABSTRACT

Using density functional theory (DFT), we have studied the structure of a zigzag silicene nanoribbons (SiNRs) with periodically embedded with four- and eight-membered rings, and studied their electronic properties by calculating its band structures and density of states (DOS). The results showed that the zigzag SiNRs have a sp^2 hybridization, in addition, the band gap gradually decreased with the increase of the width by layer, and gradually changed from semiconductor properties to metal properties. The existence of vacancy defects increased the band gap and energies, but their positions could not change the structure and the electronic properties.

1. Introduction

Graphene has been one of the most extensive subjects by scientists because of its excellent physical and chemical properties and great potential applications [1–4]. At the same time, with the further research of graphene, many non-carbene nanomaterials has been studied both experimentally [5–8] and theoretically [9–13]. Silicon (Si), one of the main members of the first-generation semiconductors and an important element of high-tech electronic devices, Because of the same main group of carbon, with four valence electrons, It has also became another hot spot for scientists to study extensively, the large quantity of work have been carried out, and it has made a considerable progress [14–18], the similarities between silicene and graphene have also been unravelled by scientists [19,20]. In addition, The application prospects of silicon-based nanoelectronics combined with the traditional semiconductor industry are very broad, which will be a field worthy of further study.

Experimentally, scientists have successfully prepared SiNRs [20–23], and there are many theoretical studies. L. Pan et al. has studied the thermoelectric properties of armchair and zigzag SiNRs based on the density functional theory [24]. S. Cahangirov et al. studied the armchair SiNRs honeycomb structures [25]. Chao Lian and Jun Ni studied the structure and electronic properties of the SiNRs on Ag (110) and found the most stable structure [26]. Based on the first principle, Song et al.

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studied the effects for SiNRs with various of width and edge shape [27], what more, they also investigated the electronic properties of the armchair SiNRs with vacancies [28].

In recent years, the structure of non-pure six-membered rings alkenes has been gradually investigated. Liu et al. studied the T graphene with the first principle, a four- and eight-membered rings graphene allotropes [29]. Zhang et al. investigated graphene allotrope consisting of five-membered rings [30]. Jorge l. Cerdá et al. studied pentagonal SiNRs aligned perfectly on Ag (110) [31]. Lin et al. calculated four- and eight-membered rings silicene with DFT [32]. In particular, Liu et al. successfully synthesized a graphene-like nanoribbons periodically embedded with four- and eight-membered rings in 2017 [33]. Considering isomorphism with different elements and structural similarity between carbon and silicon, we supposed that there should be a SiNRs embedded with four- and eight-membered rings periodically. Therefore, in this work, The structures and electronic properties of the zigzag SiNRs with different widths and vacancy defects were studied by molecular simulation. Unlike the purely six-membered rings SiNRs previously reported, this article investigated a new structure periodically embedded with four- and eight-membered rings, having a sp^2 hybridization. compared with pure six-membered SiNRs, there are some differences in the electronic properties.

2. Calculation method and detail

All the calculations in this paper were carried out using the Gaussian03 package and DFT were applied to investigated the objects. The exchange-correlation potential B3LYP [34] and the all electron 3-21G [32] basis set had been chosen. The specific calculation steps were as follows: Using periodic boundary condition (PBC), optimized the structure of H-terminated novel zigzag SiNRs, the convergence threshold was set at 10^{-6} au. Then, described energy band structures with 240 k-points in the Brillouin zone. And then, The DOS was calculated with gaussian functions while discrete peaks were set to 0.3 eV.

The structure of graphene-like nanoribbons synthesized by Liu and his co-worker was including of four-, six- and eight-membered rings. The two-dimensional planar structure of this SiNRs could be obtained by replacing carbon with silicon (Fig. 1).

In Fig. 1, the $\vec{C}_h$ is used to represent the chiral vector of the nanotubes, defined as $\vec{C}_h = k\vec{a}_1 + g\vec{a}_2$, which $\vec{a}_1$, $\vec{a}_2$ is base vector. As can be seen, the $|\vec{a}_1|$, $|\vec{a}_2|$ is not equal. When $g = 0$ or $k = 0$, rolled up the nanotubes in OA or OB direction, called zigzag nanotubes. When $k = g$, in the same method, it is along the OC direction, called armchair nanotubes. When $k \neq g$, it is

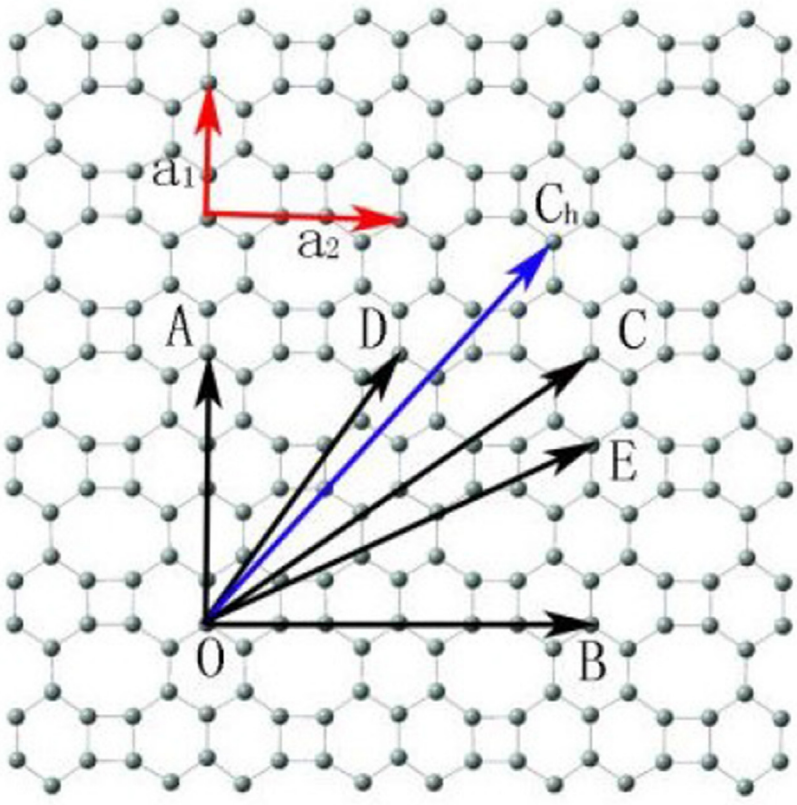

Fig. 1. The two-dimensional planar structure of SiNRs.