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Band gap engineering in Silicene NanoRibbon by hydrogen edge–termination: Atheoretical study of ab initio Density functional theory DFT

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ABSTRACT

In this work, the structural stability and electronic properties of hydrogen edge-passivated planar silicene nanoribbons (PLSiNRs) are systematically investigated using first-principles Density Functional Theory (DFT) calculations. Both zigzag (PLZSiNRs) and armchair (PLASiNRs) edge configurations are examined as a function of ribbon width to evaluate the role of edge geometry and hydrogen termination. The results reveal that hydrogen passivation effectively stabilizes the ribbon edges by eliminating dangling bond states and significantly modifies the electronic structure. Zigzag PLSiNRs–H exhibit metallic or semi-metallic behavior characterized by nearly flat edge-localized bands close to the Fermi level. In contrast, armchair PLSiNRs–H behaves as direct band gap semiconductors with width-dependent energy gaps. The band gap decreases as the ribbon width increases due to quantum confinement effects and follows the three-family behavior Eg(3n+1) > Eg(3n) > Eg(3n+2). Formation energy calculations confirm the thermodynamic stability of hydrogen-passivated systems. The tunability of the band gap through edge engineering and width modulation highlights the potential of planar silicene nanoribbons for nanoelectronic and field-effect transistor applications.

KEYWORDS

Density functional theory
Electronic properties
Silicene NanoRibbon
Localized edge state

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1 Introduction

Silicene, graphene's cousin is considered to be monolayer of silicon atoms in honeycomb structure has attracted plenty of attentions in the field of 2D materials in recent years [1]. Contrary to graphene, silicene is not absolutely planar, it has three types of honeycomb structures (planar (PL), low-buckled (LB), and high-buckled (HB)). Several groups confirmed that the silicene to be stable in the low-buckled honeycomb structure [2]. They also showed that the low-buckled (LB) and the planar (PL) are zero-gap semiconductors (or semimetals) with a linear dispersion and a Dirac cone at the K and K'points in the Brillouin zone. These characteristics are responsible for observed high charge-carrier mobility and a better controllability of the energy gap, which are necessary for transistor applications [3]. In order to realize the potential of silicene for novel electronic devices applications in the semiconductor industry, inducing and tuning its band gap is a fundamental necessity. One of the popular ways to reduce the band gap in silicene is achieved by tailoring silicene sheet into nanoribbons (SiNRs) [2]. SiNRs are classified into two basic edge types; zigzag-edged SiNRs (ZSiNRs) and armchair-edged SiNRs (ASiNRs) [4]. The structural size and geometry (edges and width) of these two types SiNRs play an important role for the future applications of Si nano-devices. For example, the edges of LBSiNRs exhibited strong resistance towards oxidation [5].

Recently, manipulating the structural size and geometry of LBSiNRs [6] play the major role to tailor the electronic and magnetic properties of these systems. On the other hand, due to their small sizes, the width and edge structure of the SiNRs are difficult to control during the experimental realization. It is currently believed that edge-Chemistry passivation is an effective way to overcome this problem and is one of the most popular choices to tailor the properties of various NRs. For example, a recent DFT calculations suggested that the LBNRs such LBSiNRs [7] and germanene nanoribbons (LBGeNRs) [8] can be easily passivated with hydrogen element, which offer more stable structures than other passivated atoms in most cases. It was found that the LBASiNR or LBAGeNRs passivated by hydrogen atom are nonmagnetic semiconductors depend on their width. While the LBZSiNRs or LBZGeNRs can be converted into a spin gapless semiconductor (SGS), ferromagnetic metals or half-metals along their edges. However, the investigation of the effect of edge passivation with hydrogen atom on the geometry, stability and electronic properties of the PLSiNRs is still absent. To address this issue, in this work, utilizing the first-principles approach based on DFT, we aim to study the impacts of H-passivation on the Stability and electronic properties of the bare PLSiNRs (without H- edge passivation) with either zigzag or armchair edges on both sides. We address the following questions: what is the influence of the structural size and geometry (edge shape and width) on the properties PLSiNRs? How do the electronic structures of PLSiNRs change with hydrogen H as a passivating element on the edge? Can PLSiNRs be rendered semiconductor depending on their edge type shape, width and edge passivation? The results show that this H-edge passivation can be used to evaluate the stability of the bare PLSiNRs. And these size and geometry-dependent systems with H- edge passivation could be potential in FET applications.

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2 Method and Model

The structural optimization and electronic properties of planar silicene nanoribbons (PLSiNRs) were investigated within the framework of Density Functional Theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP) [9]. The electron–ion interactions were described using ultrasoft pseudopotentials [10], which provide an efficient and accurate treatment of valence electrons while reducing the required plane-wave basis size. The Si $3s^2 3p^2$ and H $1s^1$ electrons are treated as valence electrons DFT. The exchange–correlation effects were treated within the generalized gradient approximation (GGA) using the Perdew–Wang 1991 (PW91) functional. The GGA-PW91 functional is well suited for describing the bonding characteristics and electronic behavior of silicene-based nanostructures [11]. A plane-wave cutoff energy of 500 eV was employed to ensure the convergence of total energies and electronic structures. Brillouin zone integrations were performed using Monkhorst–Pack k-point meshes of 10 × 1 × 1 for structural optimization and 21 × 1 × 1 for electronic band structure calculations. These k-point samplings are appropriate for one-dimensional periodic systems and were verified to provide converged results. All geometries were fully relaxed until the total energy difference between successive ionic steps was less than 10^{-5} eV, while the Hellmann–Feynman forces acting on each atom were below 0.05 eV/Å. To eliminate artificial interactions between neighboring periodic images, a vacuum spacing of 15 Å was introduced perpendicular to the ribbon plane.

All calculations were performed within a non-spin-polarized framework, since the primary objective of this work is the investigation of hydrogen-passivation-induced band gap modulation and structural stability in planar silicene nanoribbons. Hydrogen edge termination tends to suppress dangling-bond-related magnetic instabilities; therefore, non-spin calculations provide a reasonable description of the studied systems.

In our calculations, all hydrogen edge- passivated planar SiNRs are denoted as Nz–PLSiNRs–H and N_a–PLSiNRs–H, where "N" the nanoribbon width, is the number of Si dimer lines and zigzag Si chains across the ribbon's width for both armchair (a) and zigzag (z) edges, respectively. As examples, the schematic atomic structure models of bare PLSiNRs (without H- edge passivation) 5–PLZSiNRs and 7–PLASiNRs are shown in Figure 1(a) and (b), respectively.

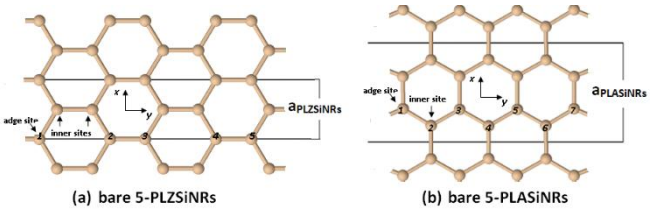

Fig. 1. The schematic atomic structure of bare PLSiNRs (a) 5–Z SiNRs and (b) 7–ASiNRs. The Brown balls represent Si atoms. The area between two black lines represents the lattice constant of PLSiNRs.

3 Results and Discussion

3.1 Geometrical stability

In order to understand the impacts of hydrogen - passivation on the geometry, stability and electronic properties of planar PLSiNRs with either zigzag or armchair edges on both sides, we investigated H edge–passivated PLSiNRs (PLSiNRs-H) with the width Nz/ Na = 2–14 for the PLZSiNRs and PLASiNRs types. We first discuss the geometrical properties of PLZSiNRs-H and PLASiNRs systems, we choose the width of Nz = 5 and Na=7 for Nz -PLZSiNR-H and Na-PLASiNR–H, respectively, as a representative in this study. The geometries of 5–PL ZSiNR–H and 7– PLASiNR–H are presented in Figure 2(a) and (b), respectively. Structural and electronic parameters such as the lattice constants (a), average silicon –silicon bond length LSi–Si, average silicon edge–H bond length LSi–H, H–Si–Si angle edge ($ø_H$), and the band gaps Eg of planar 5–PLZSiNR–H and 7-PLASiNR–H are presented in Figure 2(a) and (b), respectively. The formation energy Ef for per atom is defined by Ef = (ENz/Na-PLASiNR–H –EZ/ASiNR + n EH2/2) /n, where ENz/Na–PLSiNR–H, ENz/Na–PLSiNR, EH2, are the total energies corresponding of Nz/Na-PLSiNR–H, bare Nz/Na-PLSiNR (without H-edge passivation), hydrogen molecule and n the number of hydrogen atoms attached to the edges, respectively. Very recently, a study of the LBZSiNRs was done by Aghaei, et al. [12], respectively. They predicted that these buckled materials have negative Ef values, which indicate the possibility to synthesize of these systems. As shown in Figure 2(a) and (b), planar 5-PLZSiNR-H and 7-PLASiNR-H systems also should be realized in experimentally, as evidenced by the negative E_f.

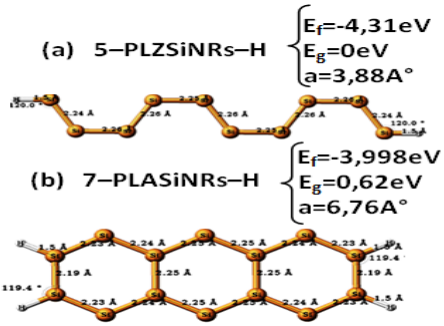

Fig. 2. Optimized lengths (Å) of Si–Si and Si–H bonds and H–Si–Si angle edge ($ø_H$) in planar (a) 5–PLZSiNR and (b) 7–PLASiNR terminated with H atoms. The brown and white balls represent Si and H, respectively.

A comparative analysis between planar and low-buckled hydrogenated silicene nanoribbons is presented in Table 1. The results reveal noticeable differences in their structural characteristics, including lattice constants, geometric configuration, buckling distance, Si–Si–H edge bond angles, and hybridization nature. The planar nanoribbons possess a flat honeycomb structure with zero buckling distance and Si–Si–H bond angles close to 120°, corresponding predominantly to sp^2 hybridization. In contrast, low-buckled silicene structures exhibit buckled honeycomb geometry with a finite buckling distance and smaller Si–Si–H bond angles ranging approximately from 109° to 112°, which are associated with mixed sp^2–sp^3 hybridization. This mixed hybridization originates from the finite buckling between silicon atoms and contributes significantly to the enhanced structural stability of low-buckled configurations compared with perfectly planar structures.

Table 1. Comparative analysis of the structural characteristics of planar and low-buckled hydrogenated.

Property	PL-ZSiNR-H	PL-AiNR-H	LB-ZSiNR-H	LB-AiNR-H
2D-Geometry	Flat honeycomb structure	Flat honeycomb structure	Buckled honeycomb structure	Buckled honeycomb structure
Lattice Constant a(Å)	3.88	6.76	3.87 [12]	6.7 [12]
Si-Si –H Edge Bond angle	120	119.4	107-110 [12]	108-111 [12]
buckling distance Δ (Å)	0	0	0.44 [12]	0.44 [12]
Hybridization sp	sp^2	sp^2	sp^2+sp^3 [12]	sp^2+sp^3 [12]

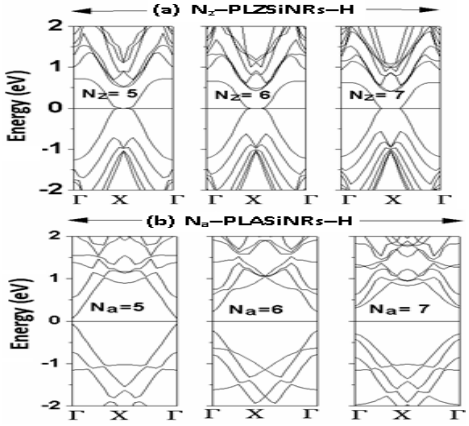

Fig. 3. The band structures of planar (a) Nz–PLZSiNR–H and (b) Na–PLASiNR–H with Nz /Na = 5–7 for. The Fermi level EF is set to zero and is indicated by the horizontal black lines.

To investigate of tuning of the electronic properties by functionalized PLZSiNR, the band structure of bare PLSiNRs and PLSiNRs–H are obtained. The band structures of Nz–PLSiNRs–H are shown in Figure 3(a). The planar ZSiNRs–H with Nz = 5–7 are taken as an example to discuss here. Our calculations show that all PLZSiNRs–H having zero gaps at the X point regardless of their widths but the energy gap at the Gamma point the band gaps are non-zero. The lowest conduction band (LCB) and the highest valence band (HVB) are always meet at one k point, so they are nearly flat bands at the Fermi level EF termed as edge states. Such a phenomena was also observed by experimental realization in zigzag graphene Nanoribbons (ZGNRs) by Nakada et al. [13] and in 2D low-buckled silicene by Feng et al. [14], where similar metallic features originate from π-edge states. On the contrary, these edge states don't show in PLASiNRs-H due to their specific dimer edge.

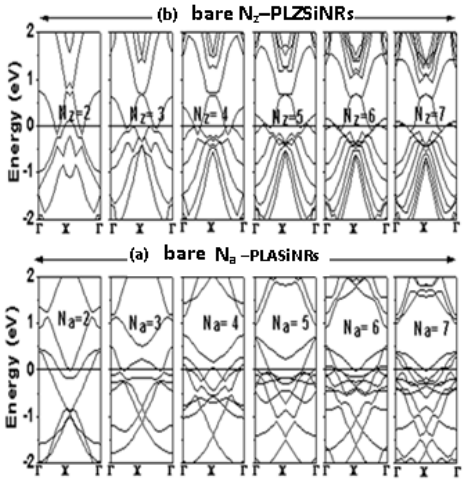

Fig. 4. The band structures of bare (a) PLZSiNRs and (b) PLASiNRs with Nz/Na = 2–7. The Fermi level EF is set to zero and is indicated by the horizontal black lines.

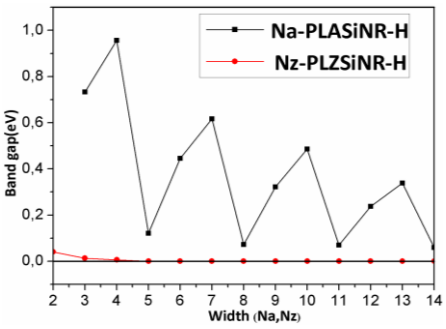

Fig. 5. Energy band gap (Eg) as a function of the width Nz(red line)/Na(black line) for PLZSiNRs –H and PLASiNRs–H, respectively.

As examples, Figure 3(b) shows the band structures of PLASiNRs–H with Na = 5–7, it can be seen the top of the valance band and the bottom of the conduction band appeared at Gamma point are always separated representing a direct semiconducting character for all PLASiNRs–H. In addition, the semiconducting energy gaps monotonically decrease with increasing ribbon widths or the numbers of the Si–Si dimer lines (Na) of the PLASiNRs–H.

As comparison studies, we also investigated the effect of the dangling bond on the electronic properties of PLSiNRs. Taken as an example the band structures of bare Nz–PLZSiNR and Na– PLASiNRs with Nz/Na = 2–7 are shown in Figure 4(a) and (b), respectively to comparing with Figure 3 (a) and (b) for the band Nz–PLZSiNRs–H and Na–PLASiNRs–H, respectively. It can be seen that several bands traversing the Fermi level accompanied with an upwards shift of all electronic energy levels, so that both bare PLZSiNRs and PLASiNRs are always exhibit metallic character independently of the width. This is in excellent agreement with the previous experimental and theoretical investigations [4, 7].

The variations of the band gap with the width Nz = 2–14 for the Nz–PLZSiNRs–H and Na = 3–14 for Na–PLZSiNRs–H are summarized in Figure 5. It can be seen the effect of edge passivation on the Eg of edge passivation on the Eg of PLZSiNRs–H is different from that of planar Na– PLASiNRs–H. The variation of band gap of the narrower than Nz = 4 are nonzero at the X point. This is because these ZSiNRs are too narrow to separate the edge states penetrating from both edges. When Nz is larger than 4, the Eg values are almost the same and close to zero regardless of their widths.

The calculated band structures indicate that hydrogen-passivated armchair silicene nanoribbons exhibit semiconducting behavior with direct band gaps. Moreover, the band gap progressively decreases as the ribbon width increases. This behavior can be attributed to the quantum confinement effect, where electrons in narrow ribbons are strongly confined within a limited transverse, leading to larger separation between the valance and conduction energy levels. As the ribbon width increases, the confinement effect weakens, allowing the energy levels to move closer to each and consequently reducing the band gap values. Clearly, the band gaps of Planar ASiNRs–H present oscillatory behavior and can be classified into three branches N=3n, 3n+1 and 3n+2, where n is an integer. The order of their band gaps sizes of –H functionalized ASiNR is Eg(3n +1) > Eg(3n) > Eg(3n +2). For example, the band gap of 6-ASiNR is 0.446 eV, those of 7-ASiNR and 8-ASiNR are 0.617 eV and 0.072 eV, respectively.

4 Conclusion

In this study, the structural stability and electronic properties of hydrogen edge-passivated planar silicene nanoribbons (PLSiNRs) were systematically investigated using first-principles Density Functional Theory (DFT) calculations. The effects of ribbon width, edge geometry, and hydrogen termination were analyzed for both zigzag (PLZSiNRs) and armchair (PLASiNRs) configurations. The obtained results demonstrate that the electronic properties of planar silicene nanoribbons strongly depend on both edge type and ribbon width. Zigzag PLSiNRs–H exhibit metallic or semi-metallic behavior due to the presence of nearly flat edge-localized bands near the Fermi level. This behavior is consistent with similar edge-state features reported in zigzag graphene nanoribbons. In contrast, hydrogen-passivated armchair PLSiNRs behave as direct band gap semiconductors. The band gap of armchair PLSiNRs decreases with increasing ribbon width as a consequence of the quantum confinement effect. Narrow ribbons exhibit stronger carrier confinement, resulting in larger energy separation between the valence and conduction bands, whereas wider ribbons show reduced confinement and smaller band gaps. Furthermore, the band gap follows the characteristic three-family behavior Eg(3n+1) > Eg(3n) > Eg(3n+2). Formation energy calculations confirm that hydrogen passivation significantly improves the thermodynamic stability of planar silicene nanoribbons by eliminating dangling bond states at the ribbon edges. Therefore, edge engineering combined with width modulation provides an efficient strategy for tuning the electronic properties of silicene nanoribbons. Overall, the present results highlight the strong potential of hydrogen-passivated planar silicene nanoribbons for future nanoelectronic and field-effect transistor (FET) applications. Future work may include effective mass calculations, transport simulations, and investigations under external electric fields or mechanical strain in order to further evaluate device-level performance.

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Declaration of Competing Interest

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