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Band gap engineering in silicene: A theoretical study of density functional tight-binding theory

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HIGHLIGHTS

- We studied the electronics properties of silicene sheet and nanoribbons.
- The band gap opens by functionalization of silicene.
- Direct band gap at K point for silicene changed to the gamma point.
- An oscillating decay occurs for the band gap of the armchair nanoribbons with increasing the nanoribbons width.
- The external electric field can open the band gap of silicene.

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ABSTRACT

In this work, we performed first principles calculations based on self-consistent charge density functional tight-binding to investigate different mechanisms of band gap tuning of silicene. We optimized structures of silicene sheet, functionalized silicene with H, CH_3 and F groups and nanoribbons with the edge of zigzag and armchair. Then we calculated electronic properties of silicene, functionalized silicene under uniaxial elastic strain, silicene nanoribbons and silicene under external electrical fields. It is found that the bond length and buckling value for relaxed silicene is agreeable with experimental and other theoretical values. Our results show that the band gap opens by functionalization of silicene. Also, we found that the direct band gap at *K* point for silicene changed to the direct band gap at the gamma point. Also, the functionalized silicene band gap decrease with increasing of the strain. For all sizes of the zigzag silicene nanoribbons, the band gap is near zero, while an oscillating decay occurs for the band gap of the armchair nanoribbons with increasing the nanoribbons width. At finally, it can be seen that the external electric field can open the band gap of silicene. We found that by increasing the electric field magnitude the band gap increases.

1. Introduction

Graphene, a 2D material, has been considered a lot of attention in recent years due to its unique electronic and mechanical properties [1–5]. For example, high carrier mobility and controllable of charge carriers of graphene make it a capable applicant for new generation electronic devices. However zero band gap value of graphene caused some problems for transistor applications [6–8]. The solution for band gap opening in the graphene can be done by functionalized it [9–11], make strain along it [12,13], to form of nanoribbons [14,15] and also by preparing defects in graphene [16–19]. Unfortunately, these structures are not very much well-matched with the existing silicon technology. As a solution, using from the other elements with the graphene-like structures has proposed [20].

Silicene, a graphene like honeycomb lattice of silicon atoms, is one of the most promoting candidate of two-dimensional material beyond graphene [21–25]. Silicene was first predicted to exist based on ab initio calculations in 1994 [21]. It has high electron mobility [26] and also it has more advantage being easily interfaced/integrated with the industrial Silicon technology [16,27–29].

In the last years silicene has been the object of many experimental and theoretical studies [30–45]. For example, silicene nanoribbons have been experimentally produced over Ag (110) surface by Padova et al. [31], silicene nanosheets have been also synthesized by Xu et al. [32] and silicene nanoribbons were successfully epitaxial grown on silver (110) and (100) surfaces by Lay et al. [34].

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Some of the theoretical investigated the mechanical and electronic properties of silicene [38–45]. For example, Topsakal et al. [38] using first-principles density functional theory studied elastic and plastic deformation of silicene nanoribbons under uniaxial tension. Botari et al. [20] investigated the mechanical properties of suspended single-layer silicone using density functional based tight-binding (DFTB), as well as reactive molecular dynamics (using ReaxFF). Also, Jing [41] studied the mechanical properties of silicone nanoribbon using DFT simulation. They showed that the Young's modulus depends strongly on the chirality and the size of the silicene nanoribbons. Song et al. [42] studied the structural and electronic properties of zigzag and armchair edge of silicene nanoribbon. Their results showed that an oscillating behavior for the armchair nanoribbons band gaps with increasing width of the nanoribbons. Berdiyorov et al. [43] studied the effect of vacancy defects on the structural properties and the thermal stability of free standing silicene by using reactive molecular dynamics simulations. Zheng et al. [44] studied the structural, electronic, and magnetic properties of saturated silicene. Finally, Kaloni et al. [45] studied a superlattice of silicene by first principles calculations. They investigated the combined effect of the intrinsic spin-orbit coupling and an external electric field, which induces a transition from a semimetal to a topological insulator and further to a band insulator.

In the present work, we have carried our simulations using density functional tight-binding (DFTB) method, for study of the silicene band gap energy with DFTB+ package. The results are organized in the five parts. The first part contains studies of band gap tuning by functionalized of silicene with F, H and CH_3 groups. The second part exhibits the effect of applying a uniaxial tension

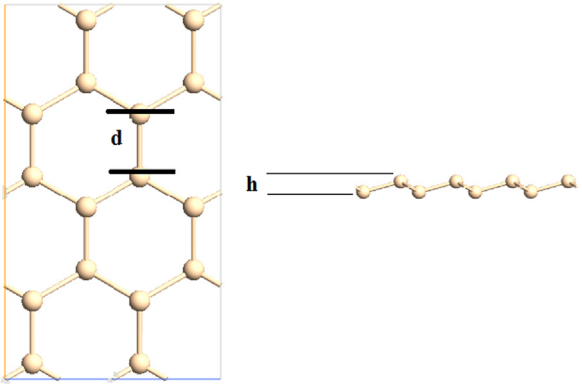

Fig. 1. Top and side view of silicene unit cell.

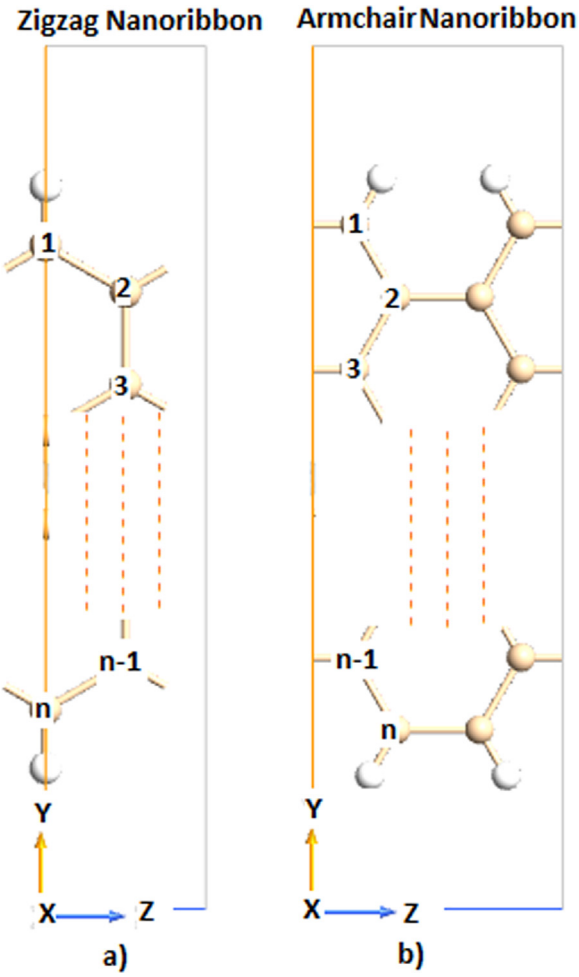

Fig. 3. The geometry structures of (a) N-ZSiNR and (b) N-ASiNR saturated with H atoms.

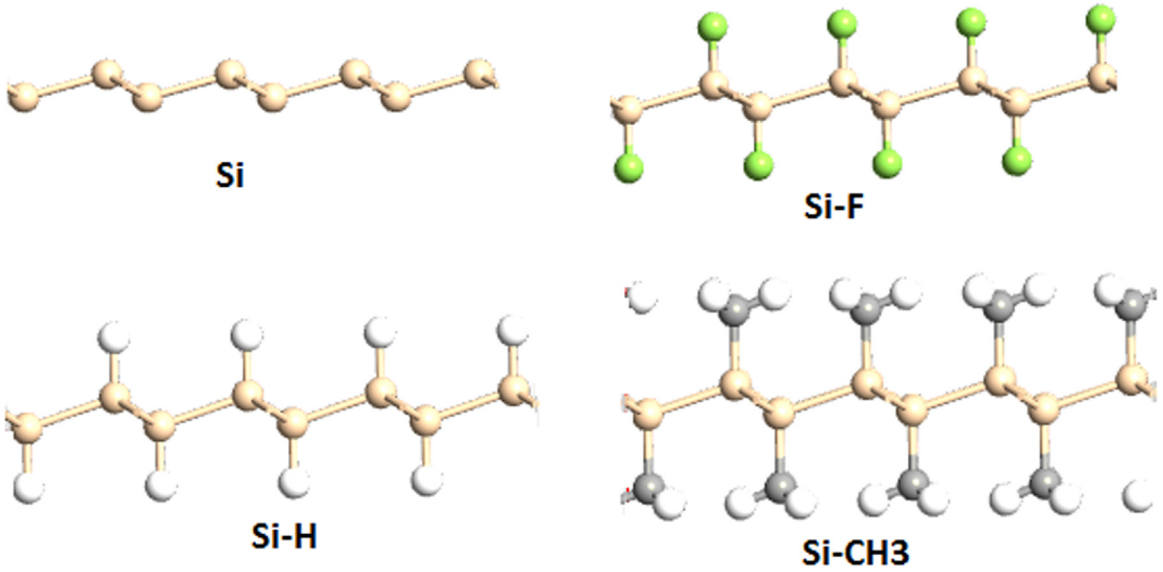

Fig. 2. The unit cell of silicene functionalized with F, H and CH_3.