

# Charge transfer of edge states in zigzag silicene nanoribbons with Stone–Wales defects from first-principles



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## ABSTRACT

Stone–Wales (SW) defects are favorably existed in graphene-like materials with honeycomb lattice structure and potentially employed to change the electronic properties in band engineering. In this paper, we investigate structural and electronic properties of SW defects in silicene sheet and its nanoribbons as a function of their concentration using the methods of periodic boundary conditions with first-principles calculations. We first calculate the formation energy, structural properties, and electronic band structures of SW defects in silicene sheet, with dependence on the concentration of SW defects. Our results show a good agreement with available values from the previous first-principles calculations. The energetics, structural aspects, and electronic properties of SW defects with dependence on defect concentration and location in edge-hydrogenated zigzag silicene nanoribbons are obtained. For all calculated concentrations, the SW defects prefer to locate at the edge due to the lower formation energy. The SW defects at the center of silicene nanoribbons slightly influence on the electronic properties, whereas the SW defects at the edge of silicene nanoribbons split the degenerate edge states and induce a sizable gap, which depends on the concentration of defects. It is worth to find that the SW defects produce a perturbation repulsive potential, which leads the decomposed charge of edge states at the side with defect to transfer to the other side without defect.

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## 1. Introduction

Currently, silicon (Si) based nanostructures, such as two-dimensional (2D) silicene, one-dimensional (1D) silicene nanoribbons, and zero-dimensional (0D) silicene clusters, are emerged as a immense interest material since their properties are similar to but richer than those of graphene [1–3]. Similar to graphene, silicene is a monolayer composed of Si atoms in a 2D honeycomb lattice and a linear dispersion near the Fermi level at the *K* point of the first Brillouin zone (BZ) makes the behavior of charge carriers as massless Dirac fermions. Contrary to graphene, the sublattice inversion symmetry can be broken due to the low-buckled geometry of silicene by applying a perpendicular electric field, leading to a sizable band gap of up to tens of meV [4–6]. Some  $sp^3$  hybridization can be found in silicene in which a large spin–orbit coupling (SOC)

are strengthened due to the buckled configuration [7]. Recently, the synthesis of silicene on different substrates, such as Ag(111) [8–11], (0001)-oriented  $ZrO_2$  on Si(111) wafers [12], Ir(111) [13], and  $MoS_2$  surfaces [14], etc., has been realized, and facilitates to further investigate the material and its properties. In comparison with graphene, silicene may be better suited for practical electronic applications since it can be more likely to integrate into Si-based electronic devices [15]. Not only silicene but silicene nanoribbons (SiNRs) have also generated much scientific interest [16–18]. Analogous to the graphene nanoribbons, SiNRs have two edge types, i.e., zigzag SiNR (ZSiNR) and armchair SiNR (ASiNR). The first principles calculations indicate that ASiNRs exhibit metals or semiconductor depending on the ribbon width and ZSiNRs show the antiferromagnetic groundstate [16]. Recent investigations have demonstrated that SiNRs, especially ZSiNRs, have rich electronic, transport, magnetic properties and may be applied in silicon-based electronic and spintronic nanodevices potentially [19–22].

The topological structural defects in graphene-based materials have been predicted to open an electronic energy band gap that can use in the design of transistors suitably [23–26]. Stone–Wales

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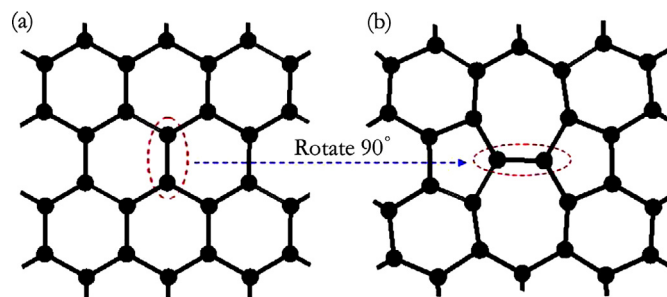
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(SW) defect is simplest topological defect which is formed by an in-plane  $90^\circ$  rotation of a bond with respect to the midpoint of the bond in 2D honeycomb lattice materials. As a result, a SW defect consists of a pair of pentagons and a pair of heptagons, and can be regarded as a dislocation (pentagon–heptagon ring) dipole [27,28]. The properties of SW defects in graphene had been investigated intensely, and this defect had been observed by a rapid quenching from high temperature or when graphene is under irradiation experimentally [29]. In silicene, some studies to understand the electronic properties, formation, stability relative to perfect silicene, and reactivity of SW defects had been presented [30]. In comparison with the formation energy of SW defects in graphene (4.66–5.82 eV) [25,31], the formation energy in silicene are found to be 1.64–2.09 eV [30,32,33], much smaller than that in graphene. It means that a SW defect can be more easily formed in silicene than in graphene. However, there have been only a few investigations on the properties of SW defects in silicene [30,32,33] and its nanoribbons [34]. In this paper, we use first-principles calculations with the density functional theory (DFT) to investigate the structural and electronic properties of SW defects with dependence on the concentration and location in edge-hydrogenated ZSiNRs. The results show that the SW defects prefer to locate at the edge due to the lower formation energy for all calculated concentrations. The SW defects at the center of ZSiNRs slightly influence on the electronic properties, however, the SW defects at the edge of ZSiNRs induce a sizable gap in the band dispersions and edge localized states are present. It is interesting to find that the SW defects at the edge results in the decomposed charge of the edge states transferring to the other side opposite of the side with defect. Our results are potentially used to design the electronic devices based on silicene in future band engineering.

Our paper is organized as follows. Section 2 briefly describes the computational methodology. In Section 3, the structural and electronic properties of SW defects with dependence on concentration of defects in bulk silicene are studied. Section 4 presents the structural and electronic properties in SW-defected ZSiNRs and their dependence on the location and concentration of defects. Finally, we conclude in Section 5.

## 2. Computational methodology

First-principles calculations are carried out within density functional theory (DFT) formalism [35,36] as implemented in the Vienna *ab initio* simulation package (VASP) [37,38]. The Kohn–Sham (KS) equations are solved self-consistently within the projector augmented wave (PAW) method [39,40] and the plane-wave basis set with a cutoff energy of 500 eV. The exchange–correlation functionals are described by local density approximation (LDA) [41] and the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) [42,43] for calculations of bulk silicene with and without SW defects, and only LDA for calculations of silicene nanoribbons. We included a vacuum region of 18 Å to avoid the interaction between the periodic layers and ribbons, respectively. In order to determine the equilibrium geometry of bulk silicene and nanoribbons with defects, all the atomic coordinates and supercell configurations are relaxed by the conjugate gradient algorithm until an energy convergence of  $10^{-6}$  eV and a force convergence of 0.01 eV/Å. The sampling of the Brillouin zone (BZ) has been done for the two-dimensional (2D) supercell with the equivalent of  $25 \times 25 \times 1$  Monkhorst–Pack [44] special  $k$ -point scheme for a bulk silicene primitive cell, and the one-dimensional (1D) supercell with the equivalent of  $25 \times 1 \times 1$  Monkhorst–Pack special  $k$ -point scheme for a silicene nanoribbon primitive cell. For the calculations of electronic density of state (DOS), the tetrahedron integration method is employed with a smearing with of 0.05 eV.



**Fig. 1.** The relaxed structures of (a) perfect and (b) SW-defected silicene. A SW defect can be created by the rotation of a silicon dimer by  $90^\circ$  around the center of the Si–Si bond (the two Si atoms in the dashed line circle).

**Table 1**

The calculated results for SW-defected silicene with respect to supercell size using both the LDA and GGA: formation energy  $E_f^{SW}$  (eV), and the length of the center Si dimer  $L_{dimer}$  (Å). The available results from the previous DFT calculations are also shown for comparison. The data in the parenthesis are the Si–Si bond length in perfect silicene.

	4 × 4	5 × 5	6 × 6	7 × 7
$E_f^{SW}$				
LDA	1.60	1.76	1.72	1.73
GGA	1.51	1.65, 2.09 [33]	1.63, 1.64 [30]	1.62, 1.82 [32]
$L_{dimer}$				
LDA (2.25)	2.18	2.16	2.16	2.16
GGA (2.28)	2.21	2.18	2.18, 2.19 [30]	2.18, 2.20 [32]

## 3. Stone–Wales defects in bulk silicene

2D honeycomb structures of Si (silicene) have been found stable in a slightly buckled geometry in DFT calculations [1] and experiments [8–14]. Due to silicene’s hexagonal structure, originated from the  $sp^2$  hybridization, the grain boundaries are expected to be formed of pentagon–heptagon pairs (i.e., a dislocation dipole), known as Stone–Wales (SW) defects. As shown in Fig. 1, a SW defect is formed by a  $90^\circ$  rotation of a Si dimer, therefore transforming a set of four hexagons into a pentagon and a heptagon pair.

The formation energy,  $E_f^{SW}$ , of a SW defect in silicene is given by

$$E_f^{SW} = E_{silicene}^{SW} - E_{silicene}, \quad (1)$$

where  $E_{silicene}^{SW}$  and  $E_{silicene}$  are the total energy of silicene with and without SW defect, respectively. We employ the supercell approach and periodic boundary condition to simulate the isolated SW defect in bulk silicene. The interaction between two SW defects is expected to be mediated by strain and long ranged because a SW defect involves a dipole of dislocation [28,31]. In order to evaluate a reasonable size of supercell in which the interaction between two SW defects would be neglected, we choose  $4 \times 4$ ,  $5 \times 5$ ,  $6 \times 6$ , and  $7 \times 7$  supercells to simulate the SW defects.

Table 1 lists the calculated results with dependence on concentration of defects in both the cases of LDA and GGA formalisms, compared with the previous available values [30,32,33]. Between the SW defects in  $4 \times 4$  and  $7 \times 7$  supercells, the differences of formation energy  $E_f^{SW}$  both for the LDA and GGA are larger than  $\sim 0.1$  eV, however those between  $5 \times 5$  and  $7 \times 7$  supercells reduce to  $\sim 0.03$  eV. Therefore, the interaction between two SW defects in  $5 \times 5$  supercell is negligible. It corresponds to the system with a defect concentration of  $2.7 \times 10^{13} \text{ cm}^{-2}$ . In the GGA formalism, the formation energy  $E_f^{SW}$  of a SW defect in a  $6 \times 6$  supercell is found to be 1.63 eV, which is a good agreement with the previous value 1.64 eV obtained by Sahin et al. [30]. However,  $E_f^{SW}$  in a  $7 \times 7$  supercell is calculated to be 1.62 eV, slightly lower than the result 1.82 eV

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