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## Research Article

# Structural Stability of Functionalized Silicene Nanoribbons with Normal, Reconstructed, and Hybrid Edges

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Silicene, a novel graphene-like material, has attracted a significant attention because of its potential applications for nanoelectronics. In this paper, we have theoretically investigated the structural stability of edge-hydrogenated and edge-fluorinated silicene nanoribbons (SiNRs) *via* first-principles calculations. Various edge forms of SiNRs including armchair edge, zigzag edge, Klein edge, reconstructed Klein edge, reconstructed pentagon-heptagon edge, and hybrid edges have been considered. It has been found that fully fluorinated Klein edge SiNRs, in which each edge Si atom is terminated by three fluorine atoms, are the most stable structure. We also discovered that a hybrid edge structure of trihydrogenated Klein edge and dihydrogenated zigzag edge can increase the nanoribbon's stability up to that of dihydrogenated armchair edge SiNR, which is known as the most stable edge-hydrogenated structure. With the attractive properties of silicene for practical applications, the obtained results will advance experimental investigations toward the development of silicene based devices.

## 1. Introduction

Since its discovery [1, 2], graphene has been found to be an attractive material owing to its wide range of applications [3–9]. Nonetheless, fabrication of graphene-based devices has been impeded by difficulties in synthesizing large area of graphene sheets, toxicity, and incompatibility with silicon-based CMOS. Silicon resembles carbon as they appear next to each other in the same group of periodic table. Recently silicene, the silicon equivalent of graphene, has captured tremendous attention since it offers similar benefits as graphene but with fewer challenges [10–14]. Numerous outstanding properties such as ferromagnetism [15], half-metallicity [16], quantum Hall effect [17], and superconductivity [18] have been reported. Silicene was first theoretically studied by Takeda and Shiraishi in 1994 [19] and then reconsidered by Guzmán-Verri and Lew Yan Voon in 2007 [20], calling it silicene. Silicene has been experimentally grown on many substrates such as Ag [21–23], Ir [24], ZrB<sub>2</sub> [25], and ZrC [26]. It possesses electronic properties similar to graphene;

for example, no band gap has been observed in silicene. The Dirac cones are also seen in silicene because of the linear crossing of the conduction and valence band at the Fermi level [27, 28]. As a result, the electron acts like massless fermions and moves through silicene with a high Fermi velocity of  $10^5$ – $10^6$  ms<sup>-1</sup> [29]. Unlike a flat graphene sheet, the stable silicene sheet is buckled [30, 31], due to the tendency of silicon atoms to accept sp<sup>2</sup> and sp<sup>3</sup> hybridization rather than sp<sup>2</sup> hybridization. The extraordinary properties of silicene along with its compatibility with silicon-based nanoelectronics give an edge to silicene over graphene in this respect. Numerous potential applications of silicene in spintronics [32], FETs [33–35], and sensing devices [36, 37] have been proposed.

One technique used to open a band gap in silicene is through silicene nanoribbons (SiNRs) [19]. SiNRs were synthesized on Ag (110) and Au (110) substrates [38–41]. It is predicted that nanoribbons can also be fabricated using nanolithography techniques [42–44]. Like graphene [45], armchair and zigzag/Klein edges are obtained by cutting

the silicene honeycomb lattice along  $\langle 1\bar{1}10 \rangle$  and  $\langle 2\bar{1}\bar{1}0 \rangle$  directions, respectively. The chiral edges are the intermediate orientations which consist of hybrid edge types. Numerous studies have been performed to explore the outstanding properties of SiNRs [46–55].

Nonetheless, so far, no in depth study has investigated the full range of SiNRs edge types. In this paper, first-principles method based on density functional theory (DFT) was employed to investigate the effects of edge hydrogenation (-H) and fluorination (-F) on the stability of different SiNRs edge types. Our results will help experimental and theoretical investigations continue to advance Si-based technology.

The paper is organized as follows. Section 2 describes the details of our first-principles calculations used to investigate the stability of SiNRs, results and discussions are detailed in Section 3, and we present our conclusions in Section 4.

## 2. Computational Methods

First-principles calculations based on DFT method are employed to perform the calculation using Atomistix ToolKit (ATK) software package [56–58]. The Perdew Burke Ernzerhof (PBE) parameterized Generalized Gradient Approximation (GGA) exchange correlation with a double- $\zeta$  polarized basis set with a mesh cut-off energy of 150 Rydberg is utilized. A vacuum space of 15 Å is employed on each side of the supercell to suppress mirroring interaction. Also, the electronic temperature was set to 300°K. All the atomic positions and lattice parameters are optimized with the maximum force and stress of 0.05 eV/Å and 0.001 eV/Å<sup>3</sup>, respectively. During optimization, a  $k$  mesh of  $1 \times 1 \times 11$  is used on our 1D structure. The  $k$  mesh is later increased to  $1 \times 1 \times 121$  to gather accurate results.

## 3. Results and Discussions

Similar to graphene [45], armchair and zigzag/Klein edges can be made from a silicene sheet by cutting along the  $\langle 1\bar{1}10 \rangle$  and  $\langle 2\bar{1}\bar{1}0 \rangle$  directions, respectively, which are called normal edges (Figure 1). Besides these edges, SiNRs with Klein edge can be reconstructed to enhance the nanoribbons' stability. As a result, a reconstructed Klein edge and reconstructed pentagon-heptagon edge will be formed. To differentiate edge structures we categorized them, similar to [59], as follows:  $a$ : armchair edge,  $z$ : zigzag edge,  $k$ : Klein edge,  $rk$ : reconstructed Klein edge, and (5-7): reconstructed pentagon-heptagon edge. Moreover, we added subscripts which show the number of functional atoms; for example,  $z_2$  indicates that all the dangling edge Si atoms are terminated by two functional atoms in the supercell. In order to separate the number of functional atoms of the two edges, we added a hyphen to the subscripts; for example,  $z_{2-1}$  shows that the edge Si atoms of one edge are terminated by two functional atoms, while on the other edge, they are attached to one functional atom in the supercell. In this paper, we have theoretically examined the stability of edge functionalized armchair, zigzag, Klein, reconstructed Klein, and hybrid edges. To investigate the effects of edge functionalization on the stability of SiNRs,  $X$

TABLE 1: Edge formation energy  $E_{\text{edge}}$  (eV) of different configurations of functionalized edge ASiNRs.

Edge type	Edge atom	$E_{\text{edge}}$ (eV/Å)
$a_{11}$	Bare	+0.33
	H	-0.08
	F	-1.03
$a_{22}$	Bare	+0.33
	H	-0.12
	F	-2.48
$a_{22-11}$	Bare	+0.33
	H	-0.02
	F	-1.75
$a_{21}$	Bare	+0.33
	H	+0.05
	F	-1.69

atoms ( $X = \text{H}$  and  $\text{F}$ ) with different densities on the edges are considered.

**3.1. Armchair Edge Silicene Nanoribbons.** Figure 2 shows different configurations of functionalized edge ASiNRs including  $a_{11}$  (mono-H or F atom on the both edges),  $a_{22}$  (di-H or -F on the both edges),  $a_{22-11}$  (di-H or -F on the one edge and mono-H or -F on the other edge), and  $a_{21}$  (both edges are periodically terminated by di-H or -F and mono-H or -F).

In order to measure the stability of functionalized edge SiNRs, we calculated edge formation energy which is described as

$$E_{\text{edge}} = \frac{(E_{\text{ribbon}} - n_{\text{Si}} \times E_{\text{Si}} - (n_X/2) \times E_{X_2})}{2L}. \quad (1)$$

Here,  $E_{\text{ribbon}}$  stands for the total energy of the functionalized edge SiNR.  $X$  is the functional addend which can be H or F atom.  $E_{\text{Si}}$  and  $E_{X_2}$  represent, respectively, the total energy of free Si and isolated hydrogen or fluorine molecule. The numbers of Si atoms and functional addends per supercell are expressed by  $n_{\text{Si}}$  and  $n_X$ , respectively.  $L$  describes the nanoribbons' periodic length and is multiplied by two because of the two nanoribbons' edge. Under perfect vacuum condition, the negative edge formation energy shows that the chemical reaction is exothermic. Table 1 presents the edge formation energies for different configuration of functionalized edge ASiNRs. As we expected, the nanoribbon with bare edges is unstable with  $E_{\text{edge}}$  of +0.33 eV/Å. Edge functionalization improves the structure's stabilities.  $a_{22}$  edged nanoribbons have the most negative edge formation energies for both the edge-hydrogenated (-0.12 eV/Å) and edge-fluorinated (-2.48 eV/Å) cases. It can be also understood that fluorination of SiNRs' edges makes the SiNRs much more stable than hydrogenation.

In order to investigate the effects of experimental conditions on the stability of SiNRs, we consider the gas pressure and temperature of the process in our calculations. To this end, we have compared the calculated edge formation energy

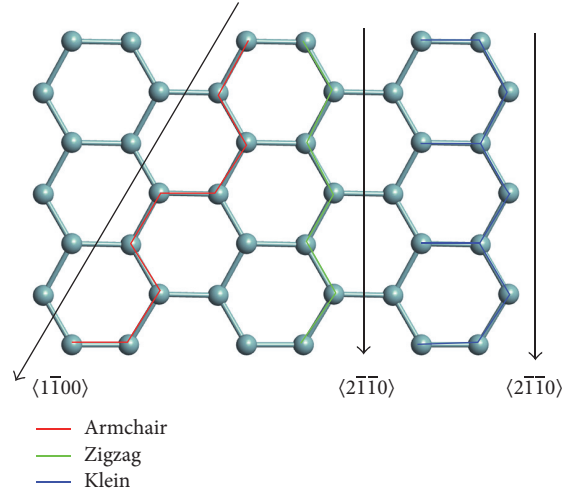


FIGURE 1: Depending on the cutting directions ( $\langle 1\bar{1}00 \rangle$  and  $\langle 2\bar{1}\bar{1}0 \rangle$ ), armchair and parallel zigzag/Klein edges can be formed by cutting silicene honeycomb sheet.

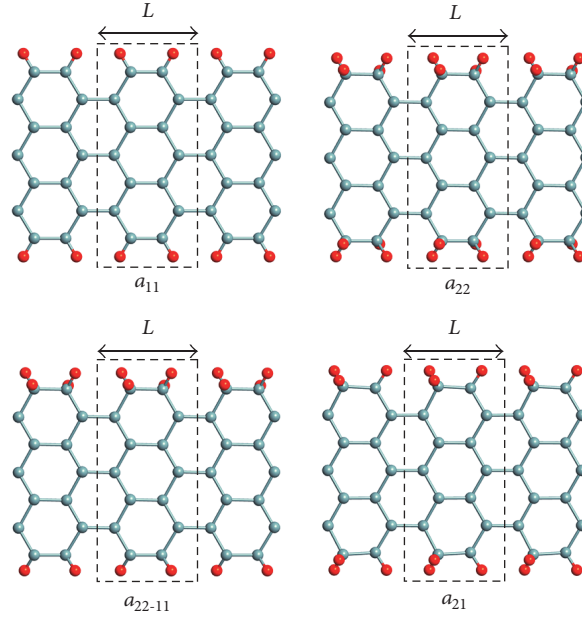


FIGURE 2: Various configurations of functionalized edge ASiNRs. The cyan and red balls represent Si and functional addends (H or F), respectively. The black dashed box shows the primitive supercell.  $L$  is the length of the supercell.

to the hydrogen or fluorine molecule's chemical potential ( $\mu_{X_2}$ ) expressed as

$$G_{\text{Func}} = E_{\text{edge}} - \frac{1}{2} \times \rho_X \times \mu_{X_2}. \quad (2)$$

Here,  $G_{\text{Func}}$  is the Gibbs free energy.  $\rho_X$  is the edge density of functional addends which is equal to  $n_X/2L$ . The temperature and gas pressure dependence ( $\mu_{X_2}$ ) is described by

$$\mu_{X_2} = H^\circ(T) - H^\circ(0) - TS^\circ(T) + k_B T \ln\left(\frac{P}{P^0}\right), \quad (3)$$

where  $H^\circ$  ( $S^\circ$ ) is the enthalpy (entropy) of functional addends at the pressure  $P^0 = 1$  bar and can be calculated using [60].

Figure 3(a) shows the values of the Gibbs free energy of  $H_2$  molecule *versus*  $H_2$  molecule's chemical potential for different configurations of functionalized edge ASiNRs. When  $\mu_{H_2}$  is less than  $-1.4$  eV,  $a_{11}$  is the most stable structure. Whereas, once  $\mu_{H_2}$  is greater than  $-1.4$  eV,  $a_{22}$  becomes the most stable one. Furthermore, under ambient conditions ( $T = 300$  K,  $P = 5 \times 10^{-7}$  bar, and  $\mu_{H_2} = -0.7$  eV),  $a_{22}$  has the most negative value of energy. For fluorinated edge ASiNRs (see Figure 3(b)),  $a_{22}$  is found as the most stable structure for the whole range of chemical potentials.

**3.2. Zigzag, Klein, Reconstructed, and Hybrid Edge Silicene Nanoribbons.** As shown in Figure 1, cutting a silicene sheet

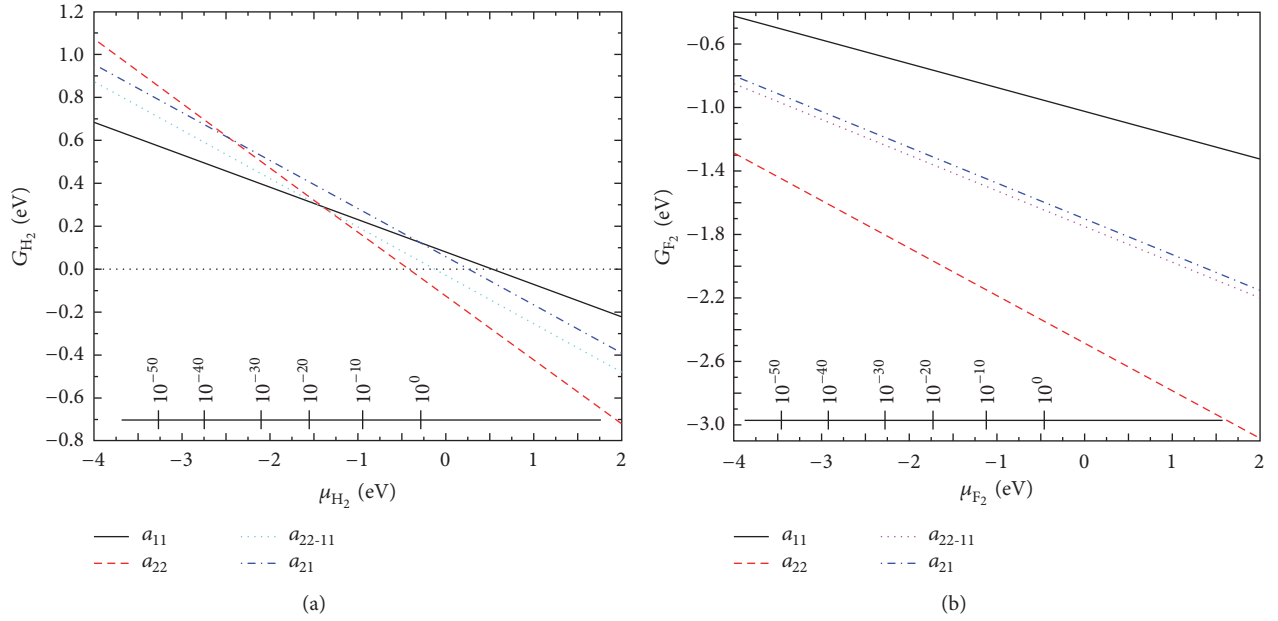


FIGURE 3: Gibbs free energy of (a) hydrogenated and (b) fluorinated edge ASiNRs as a function of chemical potential. The bottom inset axis represents the pressure (bar) of (a) molecular  $H_2$  corresponding to  $\mu_{H_2}$  and (b) molecular  $F_2$  corresponding to  $\mu_{F_2}$  when  $T = 300$  K.

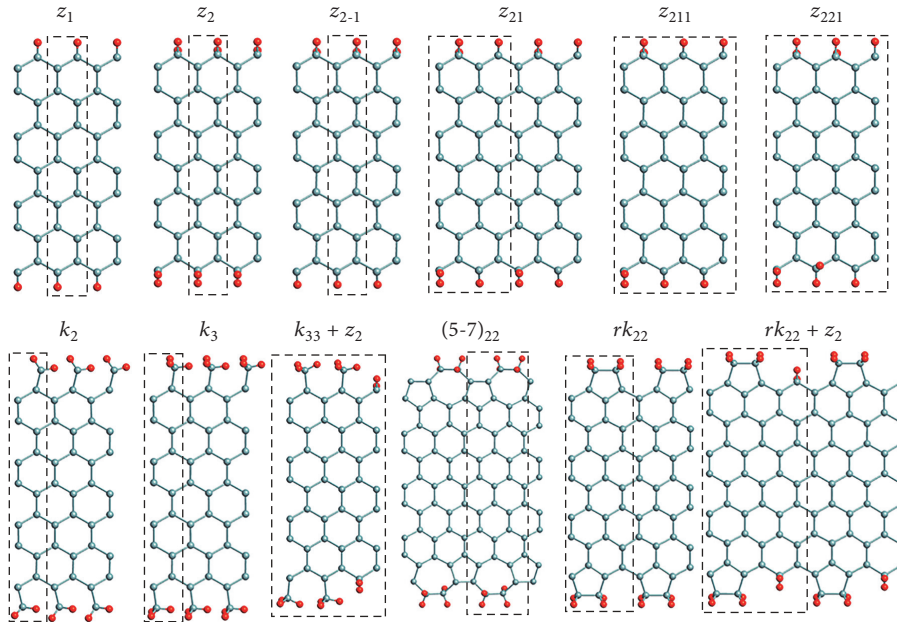


FIGURE 4: Various edge functionalized SiNRs along  $\langle 2\bar{1}\bar{1}0 \rangle$  direction. The cyan and red balls represent Si and functional addends (H or F), respectively. The dashed boxes show the primitive supercells.

along the  $\langle 2\bar{1}\bar{1}0 \rangle$  direction makes it possible to have two parallel zigzag and Klein edges. As a result, the  $\langle 2\bar{1}\bar{1}0 \rangle$  orientation is expected to be more complex than  $\langle 1\bar{1}10 \rangle$ . Different configurations of functionalized edge SiNRs along  $\langle 2\bar{1}\bar{1}0 \rangle$  direction including normal edge (zigzag and Klein), reconstructed edge (reconstructed Klein and reconstructed pentagon-heptagon), and hybrid edge structures (mixture of edges) are evaluated in this study, as shown in Figure 4. The

edge formation energies of  $z_1$ ,  $z_2$ ,  $z_{2-1}$ ,  $z_{21}$ ,  $z_{211}$ , and  $z_{221}$  are listed in Table 2. Similar to ASiNRs, the bare ZSiNRs are unstable. Through edge functionalization, the stabilities of the ZSiNRs are increased. The fully hydrogenated ZSiNR ( $z_2$ ) with edge formation energy of  $-0.01$  eV/Å is found as the most stable ZSiNR. Since Si atoms tend to accept  $sp^3$  hybridizations over  $sp^2$  in silicene, the edge formation energy increases by full functionalization of Si edge atoms. Therefore,



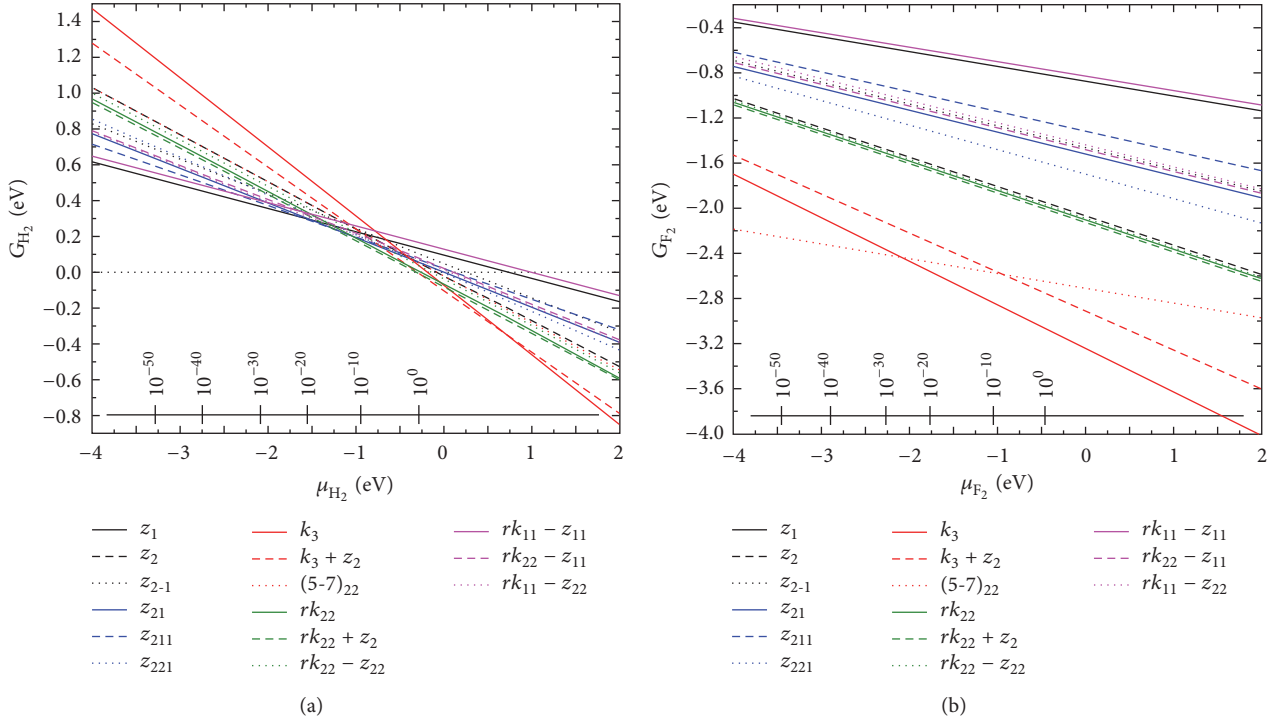


FIGURE 5: Gibbs free energy of different edge structures of (a) hydrogenated and (b) fluorinated SiNRs along  $\langle 2\bar{1}\bar{1}0 \rangle$  versus chemical potential. The bottom inset axis represents the pressure (bar) of (a) molecular  $H_2$  corresponding to  $\mu_{H_2}$  and (b) molecular  $F_2$  corresponding to  $\mu_{F_2}$  when  $T = 300$  K.

the monohydrogenated ZSiNR ( $z_1$ ) has the lowest stability among the ZSiNRs. In a similar manner to ASiNRs, fluorinating would raise the stability of the ZSiNRs ( $-2.06$  eV/Å).

The positive value of edge formation energy for bare Klein edge SiNR ( $+0.38$  eV/Å) confirms that it is unstable. It is discovered that even dihydrogenating of SiNRs' Klein edge keep them unstable ( $+0.25$  eV/Å). However, trihydrogenated  $k_3$  is fairly stable ( $-0.72$  eV/Å) due to the  $sp^3$  hybridization of Si edge atoms. On the other hand, fluorination will result in stable  $k_2$  ( $-1.85$  eV/Å) and high stable  $k_3$  ( $-3.24$  eV/Å) SiNRs. Therefore, the trifluorinated Klein edge SiNR is the most stable structure among all the edge structures (see Table 2). We have also studied different forms of Klein/zigzag hybrid SiNRs. It is found that the edge formation energy of hydrogenated  $k_{33} + z_2$  (periodic Klein vacancies which are fully functionalized by two H atoms) is  $-0.10$  eV/Å, very close to that of hydrogenated  $a_{22}$  ( $-0.12$  eV/Å). As previously mentioned, reconstruction of bare Klein edges is possible due to its high instability. Our calculations show that bare reconstructed Klein edge ( $rk$ ) and reconstructed pentagon-heptagon zigzag edge (5-7) are a slightly more stable than that of bare Klein edge (See Table 2). The monohydrogenated  $rk$  and (5-7) are still unstable; however, full hydrogenation of edges makes them stable. Interestingly, the edge formation energies for mono- and difluorinated  $rk$  and (5-7) are all negative, showing that they are all stable. The values of edge formation energies for fluorinated (5-7)<sub>22</sub> and  $rk_{22}$  are  $-2.07$  eV/Å and  $-2.10$  eV/Å, respectively. The stability of  $rk_{22}$  can be increased by periodically inserting a Klein

edge vacancy and terminating it by two functional addends, making  $rk_{22} + z_2$  structure. The hydrogenated (fluorinated)  $rk_{22} + z_2$  is  $0.01$  eV/Å ( $0.016$ ) more stable than  $rk_{22}$  (see Table 2). In conclusion, the fluorinated  $k_3$  and hydrogenated  $k_{33} + z_2$  were found to be the most stable structures along the  $\langle 2\bar{1}\bar{1}0 \rangle$  direction under perfect vacuum conditions.

In consideration of experimental conditions, the Gibbs free energies of the hydrogenated edge structures along the  $\langle 2\bar{1}\bar{1}0 \rangle$  direction were calculated using (2) and (3) (Figure 5(a)). For  $\mu_{H_2}$  is less than  $-1.5$  eV,  $z_1$  has the most negative energy. When  $-1.5$  eV  $\leq \mu_{H_2} < -0.2$  eV,  $rk_{22} + z_2$  is the most stable structure. For  $-0.2$  eV  $\leq \mu_{H_2} < +0.75$  eV,  $k_3$  and  $k_{33} + z_2$  have same Gibbs free energy. And finally, when  $\mu_{H_2} \geq +0.75$  eV,  $k_3$  is established as the most stable edge structure. Instead for fluorine, for  $\mu_{F_2} < -2$  eV, (5-7)<sub>22</sub> structure and, for  $\mu_{F_2} \geq -1.9$  eV,  $k_3$  are found as the most stable structures (see Figure 5(b)). Under ambient conditions, that is, 300 K and  $5 \times 10^{-7}$  bar, the hydrogenated  $rk_{22} + z_2$  ( $\mu_{H_2} = -0.7$  eV) and fluorinated  $k_3$  ( $\mu_{F_2} = -0.9$  eV) are the most stable edges.

#### 4. Conclusion

In summary, first-principles simulations based on DFT have been performed to study the stability of various configurations of edge-hydrogenated and fluorinated SiNRs. All possible edge types such as armchair, zigzag, Klein, reconstructed Klein, reconstructed (5-7), and hybrid edges are

TABLE 2: Edge formation energy  $E_{\text{edge}}$  (eV) of hydrogenated and fluorinated SiNRs along  $\langle 2\bar{1}\bar{1}0 \rangle$ .

Edge type	Edge atom	$E_{\text{edge}}$ (eV/Å)
$z_1$	Bare	+0.38
	H	+0.097
	F	-0.87
$z_2$	Bare	+0.38
	H	-0.01
	F	-2.06
$z_{2-1}$	Bare	+0.38
	H	+0.05
	F	-1.46
$z_{21}$	Bare	+0.37
	H	+0.001
	F	-1.51
$z_{211}$	Bare	+0.35
	H	+0.024
	F	-1.31
$z_{221}$	Bare	+0.38
	H	-0.002
	F	-1.70
$k_2$	Bare	+0.38
	H	+0.25
	F	-1.85
$k_3$	Bare	+0.38
	H	-0.72
	F	-3.24
$k_{33} + z_2$	Bare	+0.33
	H	-0.10
	F	-2.90
$(5-7)_{22}$	Bare	+0.35
	H	-0.02
	F	-2.07
$rk_{22}$	Bare	+0.33
	H	-0.07
	F	-2.10
$rk_{22} + z_2$	Bare	+0.33
	H	-0.08
	F	-2.12

studied. Results indicate that, by fluorination of SiNRs' edges, the stabilities tend to increase. Among all ASiNRs,  $a_{22}$  has the highest chance of forming both experimentally under ambient conditions and theoretically under perfect vacuum conditions, no matter the functional addends. Along the  $\langle 2\bar{1}\bar{1}0 \rangle$  direction, finding the most stable structure is more complicated than that of  $\langle 1\bar{1}10 \rangle$ . Functionalization of edge atoms by hydrogen makes  $k_{33} + z_2$  and  $rk_{22} + z_2$  the most stable structure under perfect vacuum and experimental ambient conditions, respectively. Finally, with fluorine as the functional addend,  $k_3$  structure is formed under both experiment and vacuum conditions. It should be noted that

other edge configurations can be obtained by changing the gas pressure and temperature under experimental conditions.

## Competing Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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