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Spin-semiconducting properties in silicene nanoribbons

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We have investigated the relative stabilities and electronic properties of silicene nanoribbons with sawtooth edges (SSiNRs) by first principles calculations. The SSiNR is more stable than the zigzag silicene nanoribbon (ZSiNR) and has a ferromagnetic ground state with an intrinsic energy gap between majority and minority spin-polarized bands, which shows that SSiNR is a spin-semiconductor. Under external transverse electric field, the energy gap decreases and even vanishes. Meanwhile, the charge densities of the two edge bands near the Fermi level become spatially separated at different edges. We find also that the electric field induced features can be achieved by a suitable uniaxial compressive strain. This can be understood from the effect of the Wilson transition. At last, the electronic structures of SSiNRs tuned by electric field and strain together are studied, showing that a small tensile strain makes the SSiNRs more sensitive to electric field. These results suggest that the electric field or/and strain modulated SSiNRs have potential applications in silicon-based spintronic nanodevices.

1 Introduction

Silicon-based nanoelectronics is highly promising for its compatibility with conventional semiconductor industry. One-dimensional silicene nanoribbons (SiNRs), a counterpart to graphene nanoribbons (GNRs), have been synthesized on a silver surface with a unique structure^{1,2}. Also properties of silicene nanoribbons (SiNRs) and two-dimensional silicene sheets have been investigated by the first-principles methods^{3–6}. Similar to graphene nanoribbons (GNRs)^{7,8}, SiNRs with the armchair edges (ASiNRs) are semiconductors^{3,6}, and those with the zigzag edges (ZSiNRs) have stable antiferromagnetic states, which become half-metals under a suitable external transverse electric fields³. These spin dependent properties show that silicene based nanostructures have potential applications in spintronic devices based on silicon materials.

Half-metal, in which the carriers can be fully spin-polarized with only one spin state conducting, is an typical material in spintronics^{8,9}. Another instance is spin semiconductor or spin gapless semiconductor^{10–13}. In spin (spin gapless) semiconductors, there is a (zero) energy gap between two different spin states. Thus the carriers are also fully spin-polarized with either electrons conducting one spin or holes conducting another spin. This is significant in designing qubits for quantum computing, data storage, and coding or decoding. Recently, the spin-semiconducting property in GNRs has been reported¹⁴, which enriched spintronic materials based on graphene.

In this paper, we predict the spin-semiconducting properties of silicene nanostructures. Contrasted to the sawtooth graphene nanoribbons (SGNRs), our calculations confirm that the stabilities of the sawtooth silicene nanoribbons (SSiNRs) are superior to those of the zigzag silicene nanoribbons (ZSiNRs). Under a lower electric field than that applied in SGNRs¹⁴, the SSiNRs become spin gapless semiconductors. Meanwhile, the charge densities of two opposite spin states near the Fermi energy become separated at different edges, which implies another degree of freedom in manipulating and controlling spins in silicon-based spintronics. Interestingly, a suitable uniaxial compressive strain along periodic direction in SSiNRs can also lead to spin gapless semiconductors and charge separation in real space. In addition, electronic structures of SSiNRs tuned by electric field and strain together are also investigated. These findings suggest potential applications of silicene nanoribbons in spintronic nanodevices.

2 Methodology

Using Lieb's theorem¹⁵ and a unified geometric rule¹⁶, two kinds of novel SiNRs, which are different from ASiNRs and ZSiNRs, are constructed, as shown in Fig. 1(a). Similar to GNRs¹⁶, the structures illustrated in Fig. 1(a) are called as Christmas-tree silicene nanoribbon (CSiNR) and tree-saw silicene nanoribbon (TSiNR), respectively. Both are named as sawtooth silicene nanoribbons (SSiNRs) for their edges resembling sawteeth. Two integers (n_1 , n_2) are used to label the size of the primitive cell. For CSiNRs the two integers are the numbers of hexagonal rings along the n_1 and n_2 directions. For TSiNRs n_1 is the number of continuous zigzag chains while n_2 is the number of hexagonal rings along the

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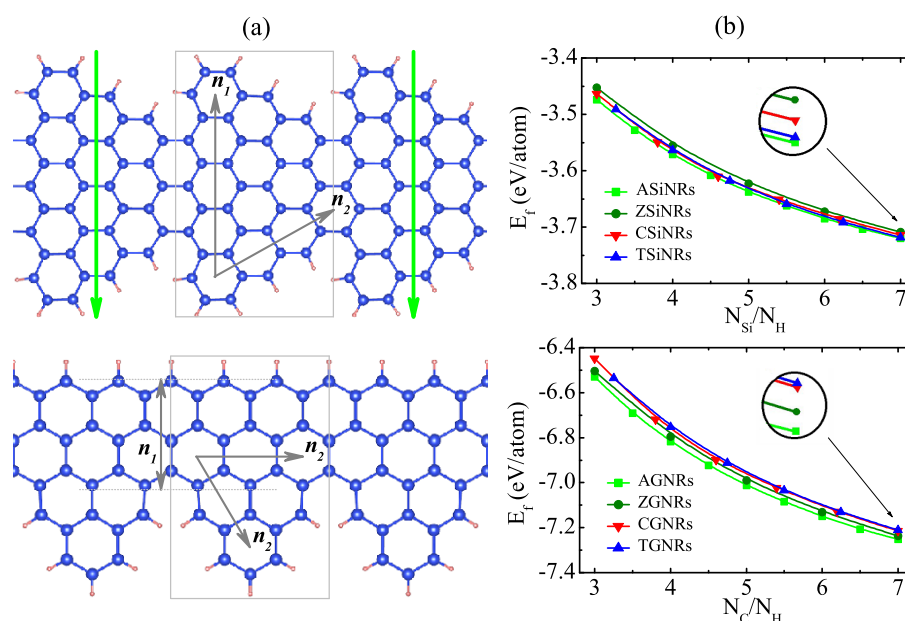


Fig. 1 (Color online) (a) Structures of a Christmas-tree silicene nanoribbon (CSiNR) (top) and a tree-saw silicene nanoribbon (TSiNR) (bottom). (n_1, n_2) denotes the size of the structures. The unit cells are marked by the gray rectangle lines. The downward bold gray (green) arrow labels the transverse electric field E_{ext} applied across the CSiNR. (b) The formation energies vs the value of N_{Si}/N_H (N_C/N_H) for silicene nanoribbons (graphene nanoribbons). The square, circle, del, and triangular lines represent the E_f of ASiNRs (AGNRs), ZSiNRs (ZGNRs), CSiNRs (CGNRs), and TSiNRs (TGNRs), respectively.

n_2 direction, as shown in Fig. 1(a). To describe them simply, we denote CSiNRs or TSiNRs of size (n_1, n_2) as $C(n_1, n_2)$ or $T(n_1, n_2)$. Figure 1(a) shows structures of the $C(5,4)$ and $T(3,3)$ SSiNRs. All of our calculations have been carried out using VASP code¹⁷. The projector augmented-wave (PAW) method¹⁸ is employed. For exchange correlation energy, the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof¹⁹ is used. The vacuum space along two aperiodic directions is larger than 15 Å. The cutoff energy is set to be 350 eV, and the structures are relaxed until all forces are smaller than 0.01 eV/Å. The tolerance of energy convergence is 10^{-5} eV. The Monkhorst-Pack k-point mesh of $(21 \times 1 \times 1)$ and $(23 \times 1 \times 1)$ are utilized to represent the Brillouin zones for the $C(n_1, 4)$ and $T(n_1, 3)$ SSiNRs, respectively. The integers $n_2 = 4$ and 3 for CSiNRs and TSiNRs, respectively, correspond to the lowest numbers meeting the requirement of the sawtooth edges¹⁶. After relaxation, the lattice constants of $C(5,4)$ and $T(5,3)$ are $a = 13.53$ Å and $a = 11.68$ Å, respectively.

3 Results and discussion

The formation energies of SSiNRs are calculated, which are used to compare with those of the armchair and zigzag silicene nanoribbons (ASiNRs and ZSiNRs) to determine the relative

stabilities of SSiNRs. From the buckled silicene hexagonal sheet^{3,20,21}, the sawtooth silicene nanoribbons (SSiNRs) are constructed. The edge silicon atoms are passivated by hydrogen atoms. The ASiNRs and ZSiNRs with the same count ratio of silicon-to-hydrogen atoms (N_{Si}/N_H) as that of SSiNRs are used for comparison. Evidently, for a given type of nanoribbons, e.g. ZSiNRs, larger silicon-to-hydrogen ratio (N_{Si}/N_H) corresponds to larger ribbon-width. The definition of the formation energies is $E_f = (E_{total} - n_{Si}E_{Si} - n_H E_H)/(n_{Si} + n_H)$. E_{total} is the total energy of SiNRs. E_{Si} and E_H are the energies of an isolated silicon atom and a single hydrogen atom, respectively. Figure 1(b) shows that the nanoribbons with larger values of N_{Si}/N_H have lower formation energies and thus are more stable than those with smaller N_{Si}/N_H values. For the ASiNRs and ZSiNRs, our results are consistent with previous work³. As plotted in Fig. 1(b), at a given value of N_{Si}/N_H , the formation energies of the CSiNR and TSiNR are lower (higher) than those of ZSiNR (ASiNR). For example, at $N_{Si}/N_H = 7$ [see inset of Fig. 1(b)] the formation energies of ASiNR, ZSiNR, CSiNR, and TSiNR are -3.720, -3.709, -3.714, and -3.718 eV/atom, respectively, indicating that the stabilities of CSiNRs and TSiNRs are between those of ASiNRs and ZSiNRs. Thus it is meaningful to investigate the properties of SSiNRs for possible applications. In comparison, we also carried out similar calculations for

graphene nanoribbons, as shown in Fig. 1(b). Differently, the sawtooth graphene nanoribbons (SCNRs) are less stable than both zigzag and armchair graphene nanoribbons (ZCNRs and ACNRs). The difference between SSiNRs and SGNRs is due to longer bond length and partial sp^3 hybridization in silicene nanoribbons.

For SSiNRs, the ground state is ferromagnetic (FM) with $2\mu_B$ magnetic moment. As shown in Fig. 2, the ferromagnetic magnetism is localized on the two edges for both kinds of SSiNRs. The energy difference between the ferromagnetic (FM) state and nonmagnetic (NM) state is about 100 meV/unit cell. The band structures of the ground state are plotted in Fig. 3(a) and Fig. 5(b) for C(5,4) and T(5,3), respectively, with one couple of spin-up bands (C_1 , C_2) above Fermi level and another couple (V_1 , V_2) below the Fermi level. The two couples of bands originate from the edge states^{14,16,22}. Between the bands V_2 and C_1 in C(5,4) and T(5,3) there is an intrinsic energy gap E_{gap} of 0.25 and 0.19 eV, respectively. These features indicate that the SSiNRs are spin semiconductors. In two dimensional silicene, A and B sublattice have identical number of atoms and occupy opposite spin states, which gives rise to antiferromagnetic property of system. However, once silicene is tailored or synthesized to the pattern of SSiNRs, the difference of the atom-number of the A and B sublattices in a primitive cell is 2. This is consistent with our results that there are two edge bands for each spin and $2\mu_B$ magnetic moment per unit cell according to Lieb's theorem¹⁵ on a bipartite lattice. Obviously, the antiferromagnetic property of primitive silicene and the edge-effect together result in the distribution of magnetism shown in Fig. 2.

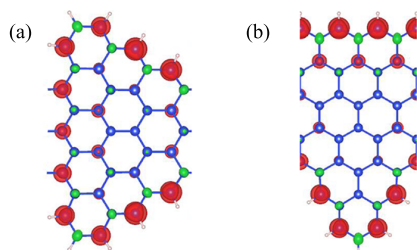


Fig. 2 (Color online) Distribution of charge density of spin-up state minus spin-down state for (a) C(5,4) and (b) T(5,3), respectively. The black (red) and gray (green) color label the spin-up and spin-down charges, respectively.

To tune the band structure and make the systems gapless spin semiconductors, we use a suitable transverse electric field since a longitudinal field can not modulate the band structure significantly. Our calculations indicate that the energy gaps in SSiNRs are sensitive to the external electric field E_{ext} whose direction is labeled in Fig. 1(a). Under E_{ext} , the edge bands with identical spins split, and the gap E_{gap} between the V_2 and C_1 bands become small. For C(5,4) and T(5,3), the gap van-

ishes at $E_{ext}=0.047$ and 0.049 eV/Å, respectively, as depicted in Figs. 3(b) and 3(e), giving rise to the spin gapless semiconductors. The carriers (electrons or holes) near the Fermi level transport in different spin states. For the geometry of C(5,4), we have made the more detailed calculations around $E_{ext} = 0$ from -0.005 to 0.005 eV/Å, which shows that the slope is zero at $E_{ext} = 0$, as shown in the inset of Fig. 3(e). This is due to the symmetry of the wavefunctions²³. Also for C(4,4), C(6,4), T(4,3), and T(6,3), we have calculated the E_{ext} inducing zero gap, concluding that a weaker E_{ext} is needed in wider SSiNRs. Notably, to get gapless spin semiconductors in SSiNRs the used E_{ext} is much weaker than that utilized in the same structures for graphene nanoribbons, such as 0.047 eV/Å in silicene C(5,4) and 0.080 eV/Å in graphene C(5,4)¹⁴. This is due to the much larger width of silicene C(5,4) than that of graphene C(5,4). However, in wider systems, e.g. C(7,4), the edge bands near the Fermi level become more flat, even under electric field inducing gapless spin-semiconducting property.

Different from half metals, the charge distribution in the SSiNRs is also separated at different edges. In the CSiNRs, the charge of each edge band localizes on both sides at $E_{ext} = 0$, as shown in Fig. 3(a). However, under $E_{ext} = 0.047$ eV/Å the charge of the V_1 and C_1 bands becomes localized on the bottom edge while those of the V_2 and C_2 are localized on the top edge, as shown in Fig. 3(b). Distinguishingly, in TSiNRs, the charges of the V_1 and C_2 localize on the top edge while V_2 and C_1 on the bottom edge at $E_{ext} = 0$, as shown in Fig. 3(c). At $E_{ext} = 0.049$ eV/Å, the charge distributions of each band of V_1 and V_2 tend to localize on both edges, but the distributions of C_1 and C_2 remain unchanged [see Fig. 3(d)]. This charge separation in real space implies that carriers transport along fixed edges according to their energy and spin states. In addition, to understand from another perspective, the DOSs of the Si 2p state at the two edges of C(5,4) with $E_{ext} = 0$ and 0.047 eV/Å are plotted in Fig. 4. At $E_{ext} = 0$, the PDOSs of the two edges are same with each other. However, external electric field makes the spin-up state of the top edge shift up and the spin-down state of the bottom edge shift down, resulting in spin gapless semiconductor at $E_{ext} = 0.047$ eV/Å. From Fig. 4 and Fig. 3(b), one can see that, for example, the DOS of the spin-up state of the top edge is mainly from the V_2 band at $E_{ext} = 0.047$ eV/Å.

Since strain is an important way to tune electronic properties^{24–29}, we also investigate the electronic properties of SSiNRs modulated by the uniaxial strain along the periodic direction. In SSiNRs, the tensile strain makes the gap E_{gap} increase slightly and the edge bands more flat. Under the compressive strain, there is a small wrinkle on the plane of ribbons. For CSiNRs this wrinkle state is metastable and its band structure is nearly same to that with no strain. However, even under a large compressive strain, e.g. $\varepsilon = -6.0\%$, the TSiNRs deform elastically. This is tested by relaxation of unloading

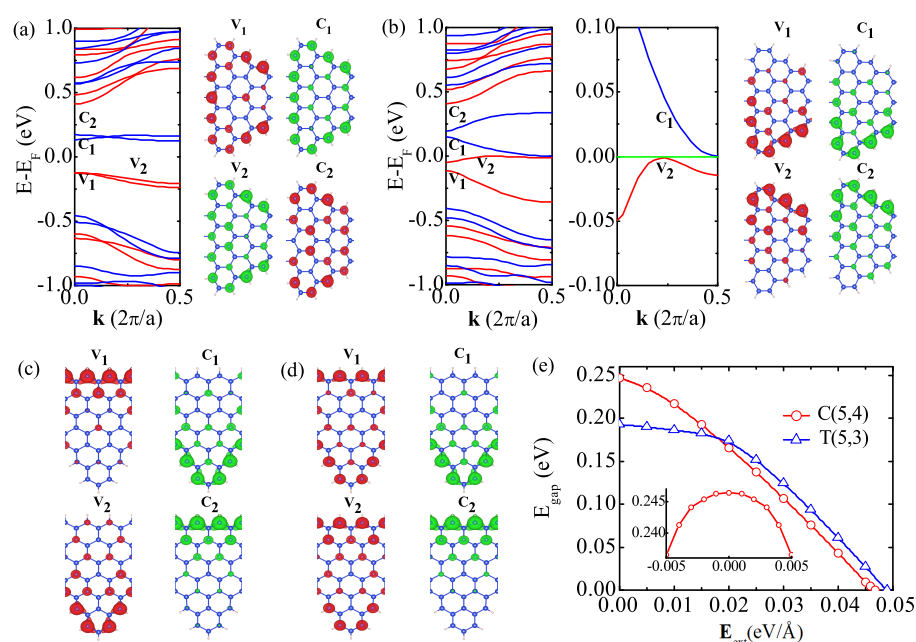


Fig. 3 (Color online) (a) Band structures and charge distributions of the edge bands V_1 , V_2 , C_1 , and C_2 for C(5,4) without electric field. (b) Same as (a) but under $E_{ext} = 0.047$ eV/Å. The right band structure is the enlargement of the left one. (c) and (d) are the charge distributions of the four edge bands for T(5,3) with electric field $E_{ext} = 0$ and 0.049 eV/Å, respectively. In band structures the black (red) and dark gray (blue) color denote the majority and minority spin states, while in charge distribution pictures the black (red) and gray (green) color label the majority and minority spin charges, respectively. (e) Energy gap of C(5,4) and T(5,3) as a function of E_{ext} . Inset shows the gap of C(5,4) near $E_{ext} = 0$.

the strains. Thus, we concentrate on the electronic properties of TSiNRs tuned by the compressive strain. Interestingly, in TSiNRs the compressive strain causes the edge bands to widen and the E_{gap} to decrease. For the T(5,3) structure the spin gapless semiconducting feature is produced at strain $\varepsilon = -4.6\%$, as shown in Figs. 5(c) and 6(a). Different from the case of applying E_{ext} [see enlarged energy band in Fig. 3(b)], the spin gapless semiconductors induced by the compressive strain have direct zero energy gap which converges at Γ point ($k = 0$), as depicted in Fig. 5(c). More interestingly, the distributions of charge density of the V_1 , V_2 , C_1 , and C_2 bands under strain are almost same to those induced by E_{ext} . After the strain $\varepsilon = -4.6\%$ is applied, the charge distribution of each spin-up edge band becomes localized on both edges while the distributions of two spin-down bands remain unchanged, as shown in Fig. 3(d). Notably, for instance, electrons on the C_1 band transport only in the spin-down state along the bottom edge while holes on the V_1 band transport along both edges. Thus, in TSiNRs tuned by E_{ext} or compressive strain, the separation of charge distribution in real space is semi-separated, which is different from that in CSiNRs.

To have an insight to strain induced change of electronic structures, we show the energy band and partial charge densities of the lowest unoccupied crystal orbital (LUCO) and the highest occupied crystal orbital (HOCO) for the T(5,3) struc-

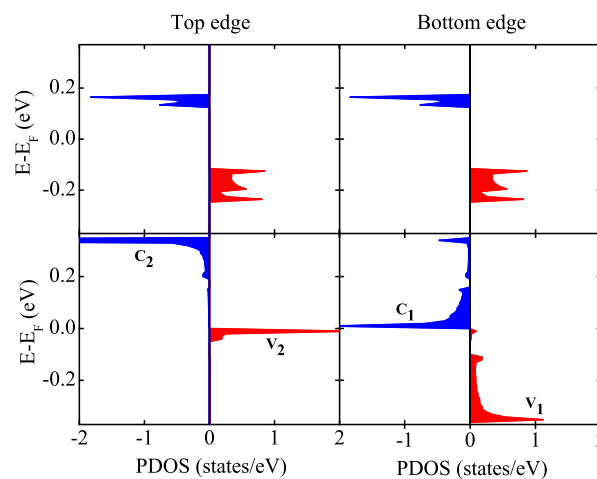


Fig. 4 (Color online) PDOS of the top edge (right) and bottom edge (left) of C(5,4) under $E_{ext} = 0$ (top panel) and 0.047 eV/Å (bottom panel), respectively. The black (red) and dark gray (blue) color denotes majority and minority spin states.

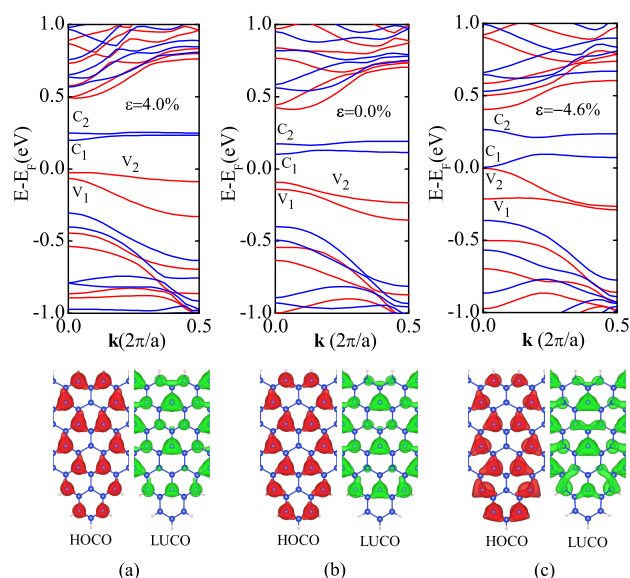


Fig. 5 (Color online) Band structures and partial charge densities of the lowest unoccupied crystal orbital (LUCO) and the highest occupied crystal orbital (HOCO) for the T(5,3) structure with the strain of (a) $\varepsilon = 4.0\%$, (b) $\varepsilon = 0.0\%$, and (c) $\varepsilon = -4.6\%$. In band structures the black (red) and dark gray (blue) color denote the majority and minority spin states, respectively.

ture with the strain of $\varepsilon = 4.0\%$, 0.0% , and -4.6% in Fig. 5. Under the above strains the LUCO and HOCO both occur at Γ point ($k = 0$). For the case of $\varepsilon = 4.0\%$, the intrinsic gap is 0.23 eV with charge density of the HOCO tending to be distributed in the upper part of the unit cell, as shown in Fig. 5(a). However, the intrinsic gap become zero under the strain of $\varepsilon = -4.6\%$, with the HOCO charge density tending to locate in the lower part of the unit cell [see Fig. 5(c)]. From tensile strain to compressive strain, the densities of both LUCO and HOCO increase slightly and become more non-localized. This phenomenon can be understood from the effect of the Wilson transition; i.e., compressive strain makes the interatomic distance decrease, then the hopping integral increase, causing non-localization of orbits, resulting in wider bands, narrowed energy gap, and even zero gap.

Now we discuss the spin gapless semiconducting properties of TSiNRs tuned by E_{ext} and strain together. Against our intuition, under the tensile (compressive) strain a weaker (stronger) electric field is needed to get zero gap, as is plotted in Fig. 6(b). In TSiNRs there is a direct gap at $E_{ext} = 0$. This direct gap decreases and turns into indirect gap as increasing of E_{ext} . Once the indirect gap is formed, the system becomes more susceptible to E_{ext} . The E_{ext} under which the transformation of direct gap into indirect gap occurs is weakened (strengthened) after applying small tensile (compressive) strains, which can be seen from the inflection point of the

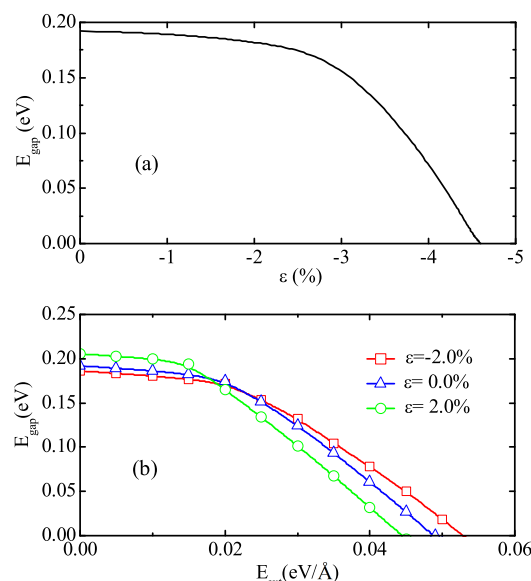


Fig. 6 (a) Energy gap of T(5,3) as a function of compressive strain. (b) Energy gap of T(5,3) as a function of E_{ext} under no strain, tensile and compressive strain, respectively.

curve of E_{gap} vs E_{ext} plotted in Fig. 6(b). From the partial charge density analysis, we concluded that under a weak tensile strain the charge of the V_2 band near $k=0.25$ and the C_1 band near $k=0.5$ become more sensitive to external transverse electric field than that without strain or with a weak compressive strain. Also a small tensile deformation makes the C-SiNRs sensitive to electric field. Thus, a small tensile strain makes the SSiNRs more sensitive to external electric field. In addition, the strain induced or strain and electric field together modulated gapless spin-semiconducting properties are also discovered in sawtooth graphene nanoribbons by our calculations. This implies another perspective to tune electric structure in spintronics based on graphene or silicene.

4 Summary

In summary, we show that different from the sawtooth graphene nanoribbons (SGNRs) the sawtooth silicene nanoribbons (SSiNRs) are more stable than the zigzag silicene nanoribbons (ZSiNRs). The SSiNRs are spin semiconductors with the ferromagnetic ground state. The spin semiconducting feature comes from the edge states. Under lower external electric field than that applying in SGNRs or suitable compressive strain, the spin gapless semiconducting properties can be achieved in SSiNRs. Besides the spin polarization in energy space, the charge distributions of the edge states also separate in real space. At last, we predicted that a tensile strain makes the SSiNRs more sensitive to electric field. These results show

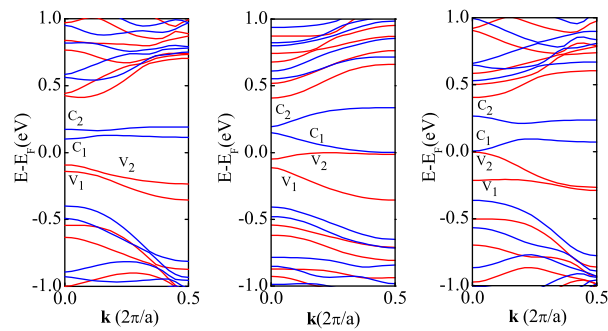
that the sawtooth silicene nanoribbons have potential applications in spintronics.

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Silicene nanoribbons with one sawtooth edge (TSiNRs) are spin-semiconductors (Left). They become spin gapless semiconductors under a suitable electric field (Middle) or a compressive strain (Right).