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Strain and chemical function decoration induced quantum spin Hall effect in 2D silicene and Sn film

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ABSTRACT

The topological properties of silicene and Sn film decorated with chemical functional groups (–H, –F, –Cl, –Br, –I) are investigated by the first-principle calculations. It is found that Sn films decorated with F, Cl, Br and I are topological insulators with sizable gap while the other combinations are normal insulators. The phase transition of X decorated silicene and Sn film was investigated by applying external strain. Our results pointed out that the normal insulators can transform into topological insulators with sizable gap under critical strain. The research provided new routes to design 2D topological insulator with sizable gap which has wide applications in next-generation spintronics devices.

1. Introduction

Recently, the subject of time-reversal-invariant topological insulators has attracted a great interest in condensed-matter physics and material science [1–5]. Topological insulators (TIs) are electronic materials that have insulating energy gaps in the bulk, but have gapless edge states and surface states that are protected by time-reversal symmetry at sample boundary [6,7]. These systems are promising sources for many exotic phenomena like Majoranan fermions [8,9] and potential applications in quantum computing and spintronics devices [10]. Usually, two-dimensional (2D) TIs have some unique advantages over three-dimensional (3D) TIs. For example, bulk carriers that often plagued their 3D counterparts can be vacated simply by gating. For 2D TIs or quantum spin Hall (QSH) insulators, the QSH state was first predicted in graphene [11,12]. However, the spin–orbit coupling in graphene was too weak to produce an observable effect at ambient conditions. Subsequently, the QSH states have been realized in several other materials, such as GaAs quantum well [6,7,13], HgTe quantum wells [14,15] and the 2D group IV honeycomb lattices like silicene, germanene and Sn monolayer [16–19]. But the QSH effect has been observed only at very low temperatures because of small bulk gaps. Recently, the QSH effect has been verified in the InAs/GaSb quantum wells by transport experiments, but there are some serious problems of very small bulk gap and incompatibility with conventional semiconductor devices. In order to realize their full potentials in experimental investigations, extensive efforts are needed to search QSH insulators with a preferable bulk gap.

Silicene has been verified to be a TI state in both theory and experiment. On account of its small bulk gap, it is difficult to be achieved in practical applications. However, silicene is still a viable TIs candidate due to its excellent properties, such as high mobility, material compatibility and easier integrability to the current electronics industry [20]. Herein, to silicene, a sizable band gap is important for practical applications. In this work, to enhance the bulk gap, silicene was decorated with chemical functional groups (–H, –F, –Cl, –Br and –I). Based on the first-principle calculations, we found that silicene decorated with chemical functional groups (X–Si, X = –H, –F, –Cl, –Br and –I) were normal insulators (NIs) with larger band gaps than that of silicene. By applying *biaxial* tensile strain, we found that X–Si can be transformed into topological phases. We also investigated phase transition by applying external strain on Sn films decorated with chemical functional groups (X–Sn). The results show that X–Sn changed from TIs into NIs under a critical compressive strain. However, further increasing the compressive strain, X–Sn transformed into topological metals (TMs). Our calculations indicate that applying external strain is a potential approach to design TIs with larger band gaps.

2. Methods

All calculations are performed within the framework of density-functional theory (DFT) with pseudopotentials formalism as implemented in Vienna ab initio simulation package (VASP) [21].

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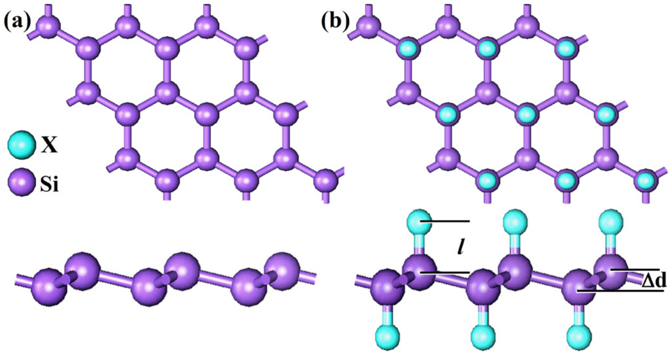

Fig. 1. The top view and side view of 3 × 3 super cells of silicene (a) and Silicene decorated X (b). The purple balls and light blue balls denote as silicon atoms and chemical functional groups X. The bonding length between I and Si atoms is defined as l, and Δd is the buckling distance between the two layers of silicon. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

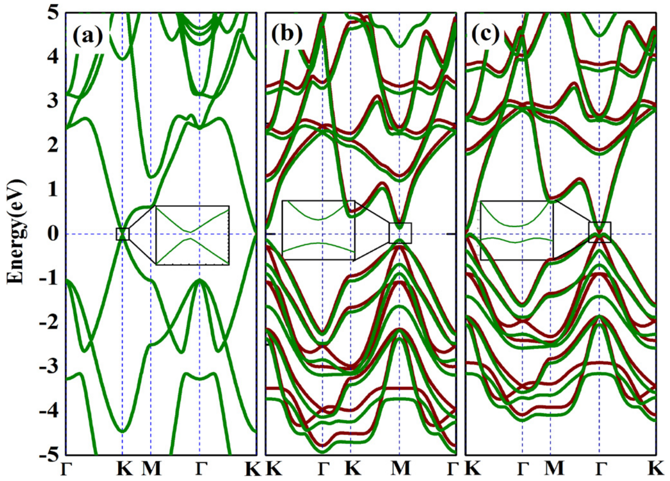

Fig. 2. Band structures of silicene (a), I–Si (b) and I–Si with external 4% tensile strain (c). Brown line is described as band structure without SOC, while green line is taken the SOC into account. Dash line at zero level is regarded as Fermi level. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The exchange-correlation function was treated using the Perdew–Burke–Ernzerhof within the generalized gradient approximation [22], and the plane-wave basis with an energy cutoff of 500 eV. In our simulations the position of all atoms were fully relaxed using the conjugated gradient method for energy minimization and the calculated force on each atom became smaller than 0.01 eV/Å. A vacuum space of 15 Å was adopted to avoid the interaction between layer and layer. The two dimensional Brillouin zone was sampled by a 15 × 15 × 1 k-grid mesh [23,24]. As these bulk gaps are influenced by the spin orbital coupling (SOC) effect, the SOC was included in the self-consistent calculations for electronic structure.

3. Result and discussion

Fig. 1 shows the optimized 3 × 3 supper cell geometries of silicene and X–Si. The silicene and X–Si are typical hexagonal honeycomb structures with their symmetric group of P-3M1 and D2D-3, respectively. The calculated lattice constants and buckling distances Δd are shown in Table 1. From Table 1, we find the buckling distance of pristine silicene Δd is 0.51 Å. Compared with the plane honeycomb structures, it is well known that the buckling in silicene weakened the π–π bonding between Si atoms and enhance the overlap between π and σ orbits. As shown in Table 1, the buckling distances of X–Si greatly enlarge. The sp^2 orbits are slightly dehybridized, forming a mix of sp^2 and sp^3 orbits in X–Si, which results in buckling structures more stable than the planar ones. The calculated lattice constants and buckling distances Δd of X–Sn are also shown in Table 1.

From the band structure of silicene as shown in Fig. 2(a), we can note that two energy bands cross linearly to form a Dirac point at the K point. However, a band gap with the value of 7.2 meV opened when the SOC was turned on. Thus, we conclude that silicene is a QSH insulator [13,15]. Our calculated result is consistent with the previous result which is based on the tight binding method by Liu [16]. In order to enhance the bulk band gap, the chemical functional groups such as –H, –F, –Cl, –Br and –I are considered to decorate silicene. As a typical example, the band structure of silicene decorated with iodine (I–Si) is shown in Fig. 2(b). Unfortunately, the Dirac point at K point suddenly disappeared because the π bonding of each silicon atom was saturated by the I atom and a large direct band gap of 0.54 eV at Γ point opened. Our results indicated that all X–Si were normal insulators (NIs). The initial phase and band gaps of X–Si were shown in Table 1. It is well known that strain is an effective means of realizing the required node-to-node transistor performance improvements [25]. Experimentally, biaxial strain can be easily implemented on the target material by touching with buffer layers [26,27]. Therefore, we studied X–Si under biaxial strain. Interestingly, under 4% tensile strain, the band structure of I–Si without SOC has a Dirac cone-character at the Γ point. However, there is an open gap about 130 meV in the band structure of I–Si with SOC as shown in Fig. 2(c). The strain is defined as $\varepsilon = (a_s - a_0)/a_0$, where a_0 is constant lattice in the 2D geometry and a_s is constant lattice with external strain [28]. Compared with the band structure of pristine silicene, our results indicated that I–Si with 4% tensile strain is a nontrivial topological insulator with a larger band gap.

Table 1
The lattice constant a (in Å), buckling distance Δd (in Å), bonding length l (in Å) between X and Si or Sn atom, the initial phase (TIs or NIs) and the energy gaps E_g (in eV) of X–Si and X–Sn.

Structure	a (Å)	Δd (Å)	l (Å)	Initial phase	E_g (eV)	Z_2/ν
Silicene	3.81	0.51	–	TIs	0.00723	1
H–Si	3.866	0.73	1.501	NIs	2.371	0
F–Si	3.964	0.705	1.634	NIs	0.7	0
Cl–Si	3.945	0.723	2.077	NIs	1.298	0
Br–Si	3.963	0.712	2.249	NIs	1.272	0
I–Si	4.064	0.69	2.477	NIs	0.54	0
Sn	4.682	0.847	–	TIs	0.092	1
H–Sn	4.721	0.784	1.742	NIs	0.241	0
F–Sn	5.012	0.529	1.969	TIs	0.294	1
Cl–Sn	4.935	0.668	2.376	TIs	0.267	1
Br–Sn	4.912	0.713	2.528	TIs	0.29	1
I–Sn	4.9	0.754	2.74	TIs	0.34	1