

Chapter 1

Physical Properties of Silicene

Lok C. Lew Yan Voon

Abstract In this chapter, we discuss the physical properties of free-standing silicene. Silicene is a single atomic layer of silicon much like graphene. The interest in silicene is exactly the same as that for graphene, in being two-dimensional and possessing a Dirac cone. One advantage relies on its possible application in electronics, whereby its natural compatibility with the current Si technology might make fabrication much more of a commercial reality. Since free-standing has not yet been made, all of the results are theoretical in nature, though most properties are not expected to differ significantly for silicene on a substrate.

1.1 Introduction

Silicene [1] is a single atomic layer of silicon (Si) much like graphene [2]. Early work, both theoretical [3–7] and experimental [8, 9], went mostly unnoticed until silicene nanoribbons were reported to have been fabricated on a silver substrate by Kara et al. in [10]. Since then, silicene sheets have been grown mainly on Ag(111) starting in 2012 [11–15]; these were achieved under ultrahigh vacuum conditions by evaporation of silicon wafer and slow deposition onto a substrate at 220–260 °C.

The interest in silicene is exactly the same as that for graphene, in being two-dimensional (2D) and possessing a Dirac cone [1]. One advantage relies on its possible application in electronics, whereby its natural compatibility with the current Si technology might make fabrication much more of a commercial reality. Indeed, a field-effect transistor made out of silicene has finally been demonstrated in 2015 [16].

L.C. Lew Yan Voon (✉)

School of Science and Mathematics, The Citadel, 171 Moultrie Street,
Charleston, SC 29409, USA
e-mail: llewyanyv@citadel.edu

In this chapter, we discuss the physical properties of free-standing silicene. Since the latter has not yet been made, all of the results are theoretical in nature, though most properties are not expected to differ significantly for silicene on a substrate. Thus, the results on free-standing silicene are relevant for studies on silicene on substrates.

1.2 Structure

Numerous theoretical studies, almost all based on first-principles calculations, of the structural properties, have been published and they are all consistent. First-principles calculations are invariably based upon density-functional theory (DFT), whether using the local-density approximation (LDA) or the generalized-gradient approximation (GGA) to the exchange-correlation potential. The local density approximation is known to lead to overbinding and, thus, a slightly smaller lattice constant.

In a DFT calculation, an initial geometry is assumed and the atoms are moved so as to minimize the total energy while preserving the lattice symmetry. Takeda and Shiraishi [4] first carried out this process for a single layer of Si. Given the already known existence of graphite, they assumed a hexagonal lattice for Si as well (with a superperiodicity perpendicular to the plane with a large vacuum layer, typically at least ~ 10 Å) and allowed the in-plane lattice constant a to vary, as well as the position of the basis atom (B in Fig. 1.1) within the unit cell while preserving the imposed D_{3d} symmetry. Realizing the fact that Si is not known to form the flat sp^2 bonding, they allowed the B atom to move out of the A atom plane. They found what they called the corrugated structure to have a lower total energy than the flat one, and a local minimum for $a = 3.855$ Å and a deformation angle of 9.9° . A more recent GGA calculation puts the lowering in energy at 30 meV/atom and a binding energy of 4.9 eV/atom, which is lower than that for bulk silicon (diamond structure) by 0.6 eV/atom [7]. As Takeda and Shiraishi pointed out [4], the corrugated structure makes sense since it resembles closely the (111) plane of bulk cubic silicon. Two ways of explaining the buckled structure instead of the flat structure of graphene are via the weakening of the π double bond due to the larger separation of the Si atoms,

Fig. 1.1 Crystal structure of silicene. The lattice is hexagonal, a unit cell is the dashed one, and the basis consists of two Si atoms labelled A and B

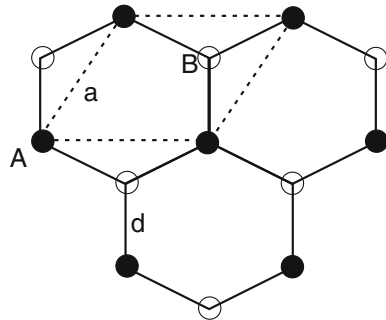


Table 1.1 Structural parameters of various 2D sheets

	d (Å)	a (Å)	Δz (Å)
Silicene [20]	2.248	3.820	0.44
Graphene [20]	1.414	2.456	
Germanene [20]	2.382	4.0	0.64
Silicon [33]	2.35		
g-Si [33]	2.35	4.07	
T-Si [33]		2.427	

and via the pseudo Jahn-Teller effect with coupling of the electronic ground state to the next one by a vibrational mode [17].

All DFT calculations since then have reproduced very similar structural parameters. Typical structural parameters are given in Table 1.1. The out-of-plane height Δz of the Si atom was found to be 0.53 Å by Ding and Ni [18], and 0.44 Å by Cahangirov et al. [19] and 0.45 Å by us [20]. In bulk Si, the out-of-plane Si atom is 0.78 Å from the (111) plane. Thus, the bonding in silicene can be viewed as in between sp^2 and sp^3 . The bond length d is much larger than for graphene because of the larger size of silicon compared to carbon.

The fact that the above structure is a local minimum in the total energy does not guarantee stability. In fact, Cahangirov et al. [19] found that silicene has another local minimum with a larger binding energy at a higher buckling, with $\Delta z \approx 2$ Å (referred to as the high buckled or HB structure compared to the low buckled or LB one). However, a variety of tests showed the LB structure to be the stable one. First, they found that, on a (2×2) supercell, the HB structure developed clustering upon structural optimization; the same group had also earlier obtained the same LB structure on a (2×2) supercell [7]. Second, both the HB and planar (PL) structures have phonon spectra with imaginary frequency modes, a signature of lattice instability. Third, the LB structure was found to be preserved upon performing ab initio molecular dynamics (MD) on a (4×4) supercell with temperature as high as 1000 K.

More recent work has questioned whether the silicene structure is, in fact, the most stable one. Thus, Kaltsas and Tsetseris [21] started with different configurations by taking the surface layer of various Si surface reconstructions and optimizing the structure. In the process, they found that structures based on the $\sqrt{3} \times \sqrt{3}$, 5×5 , and 7×7 reconstructions are actually all more stable than the perfect silicene structure, by 48, 17 and 6 meV per atom, respectively (Fig. 1.2).

In spite of the above discussions, a number of authors have explored the possibility of silicene being flat like graphene. A graphitic form of silicon, g-Si, with presumably flat silicon layers, were studied by Yin and Cohen in [22] and found to be metastable compared to the diamond structure. Based upon earlier ideas, they suggested that a pressure of -69 kbar could lead to a stable graphitic silicon. Wang et al. [5] were, on the other hand, interested in the nature of the bonding and predicted that the interlayer bonding would be stronger than the van der Waals one. As already indicated, a number of authors have compared the stability of a single

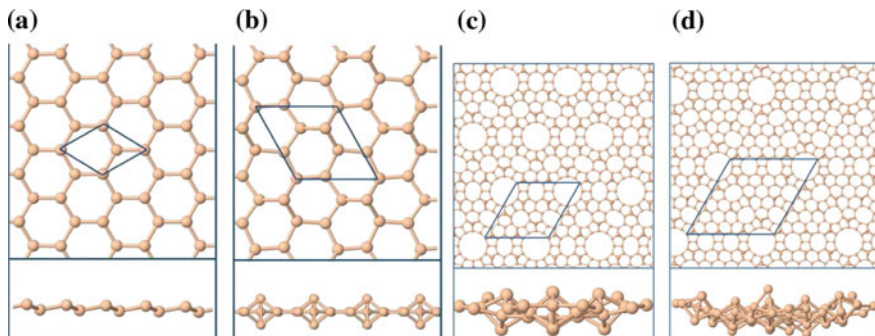
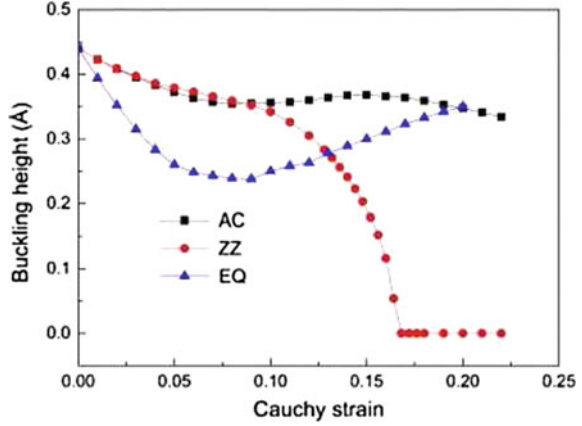


Fig. 1.2 Other possible stable forms of silicene: **a** silicene, **b** $\sqrt{3} \times \sqrt{3}$, **c** 5×5 , and **d** 7×7 . Reproduced from [21] with permission from the PCCP Owner Societies

sheet of flat silicene to that of corrugated silicene [4, 6, 7, 19]. However, a few studies assumed a flat silicene structure [23, 24], with no apparent check on the stability of such. Unfortunately, this early confusion about the structure of silicene has led to some unwarranted criticisms [25].

Nevertheless, others have looked at ways a flat sheet could be coerced to form. Three general ideas have been proposed. The first is based upon using a host to confine the Si layer [26]. Thus, an MD study using the Tersoff potential showed that liquid Si atoms confined between two parallel-plane walls separated by less than 7.5 Å can assume a flat hexagonal lattice structure when the liquid Si is quenched down from 2400 K down to 0 K [26]. The Si atoms were assumed to interact with the walls using a 9–3 Lennard-Jones potential. The stability of the structure was checked using first-principles MD up to 300 K. The second approach proposes using externally applied biaxial tensile strain [27–29]. It is very much expected that the buckling would be reduced by a biaxial tensile strain; Liu et al. [27] found it to be reduced to 0.34 Å with a 12.5 % strain. Wang et al. [29] reported that they obtained a stable flat silicene with a biaxial strain of 20 %. However, this disagrees with other studies. Thus, two groups found the buckling to reach a low (about 0.3 Å for a 10 % strain in [28] and about 0.23 Å for a 7 % strain in [30]) and then increase again (Fig. 1.3). Furthermore, a number of workers found some instability settling in around 17 % [28, 30, 31]. Yang et al. [30] proposed that a ZZ uniaxial strain of 16 % could reduce the buckling to zero but that the resulting structure is unstable from phonon calculations. The third approach for “flattening” the silicene was based on the hope that adsorption of other atoms or of a substrate might lead to a planar structure. However, functionalization studies show that the opposite happens, whereby the bonding becomes more sp^3 -like [20]. For completeness, we mention that a recent Monte Carlo calculation using Tersoff potential did not find any buckling [32], contrary to all the DFT calculations.

Fig. 1.3 Buckling parameter of silicene under external tensile strain. *AC* and *ZZ* refer to uniaxial strains (armchair and zigzag directions, respectively) while *EQ* refers to biaxial. Reprinted from [30], with permission from Elsevier [30]



1.3 Mechanical Properties

Two-dimensional materials are predicted to have much higher mechanical strengths than bulk materials [47]. Graphene is already known to have excellent mechanical strength due to its sp^2 bonding (Table 1.2). A 2D sheet should also have transversal flexibility. Additionally, the ability to support large strain means the nonlinear elastic regime can easily be attained. Thus, much of the work on mechanical properties have investigated the four regimes of linear elasticity, nonlinear elasticity, plasticity and fracture.

The elastic properties of a hexagonal 2D sheet can be characterized by elastic constants C_{11} and C_{12} , the Poisson ratio ν , and an in-plane stiffness C . If the strain energy (difference in total energy with and without strain) is assumed to depend quadratically on an external applied strain ϵ_{ij} (harmonic approximation),

$$E_s(\epsilon_{xx}, \epsilon_{yy}) = a_1 \epsilon_{xx}^2 + a_2 \epsilon_{yy}^2 + a_3 \epsilon_{xx} \epsilon_{yy}, \quad (1.1)$$

then one can show that the elastic parameters are related [34] as follows:

$$a_1 = a_2 = \frac{hA_0}{2} C_{11}, \quad (1.2)$$

$$a_3 = hA_0 C_{12}, \quad (1.3)$$

$$\nu = -\frac{\epsilon_{\text{trans}}}{\epsilon_{\text{axial}}} = \frac{C_{12}}{C_{11}} = \frac{a_3}{2a_1}, \quad (1.4)$$

$$C = hC_{11} \left[1 - \left(\frac{C_{12}}{C_{11}} \right)^2 \right] = \frac{[2a_1 - (a_3)^2/2a_1]}{A_0}, \quad (1.5)$$

Table 1.2 Physical properties of silicene compared to graphene

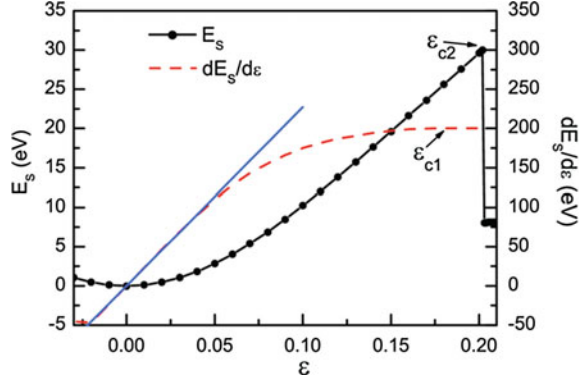
Property	Silicene	Graphene
Lattice constant ($\text{\AA}$)	3.86 [20]	2.46 [34]
Buckling ($\text{\AA}$)	0.44 [20]	0
Elastic constant C (N/m)	62 [34]	335 [34]
	60.06 (ZZ), 63.51 (AC) [35]	
	50.44 (ZZ), 62.31 (AC) [36]	
	86.48, 85.99 [37]	328.02, 328.30 [37]
Poisson ratio ν	0.30 [34]	0.16 [34]
	0.41 (ZZ), 0.37 (AC) [35]	
Young's modulus (T Pa nm)	0.178 [27]	0.420 [27]
Bending modulus D (eV)	38.63 [36]	1.5 [38]
Phonon D-mode (K point) (cm^{-1})	545 [28]	~ 1350 [39]
Phonon G-mode (K point) (cm^{-1})	550 [28]	~ 1580 [39]
Fermi velocity (m/s)	$\sim 10^5$	$\sim 10^6$
Deformation potential E_1 (eV)	2.13 [37]	5.14, 5.00 [37]
Intrinsic mobility ($105 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)		
μ_h	2.23, 2.22 [37]	3.22, 3.51 [37]
μ_e	2.58, 2.57 [37]	3.39, 3.20 [37]
Work function (eV)	4.8 [31]	4.56 [40]
Thermal conductivity κ at 300 K (W/m K)	9.4 [41]	3000–5000 [42]
Thermopower S ($\mu\text{V/K}$)	87 [43]	–32 [44]
Thermoelectric figure of merit ZT	<0.5 [45]	0.17–1.02 [46]

where h and A_0 are the effective thickness and equilibrium area of the supercell, respectively. An isotropic model is appropriate to describe the response to a biaxial strain for a hexagonal crystal. Peng et al. [47] found linear elasticity to only apply for strains smaller than 3 % in magnitude, beyond which higher-order elastic coefficients would be needed.

Sahin et al. [34] computed the Poisson ratio ν and in-plane stiffness constant C by stretching the sheets in the plane, computing the change in the total energy with the deformation, and fitting to a quadratic function. They obtained $\nu = 0.3$ and $C = 62 \text{ J/m}^2$ for silicene, compared to 0.16 and 335 J/m^2 , respectively, for graphene. The bulk modulus of silicene is reported to be 3.5 times smaller than for graphene [48]. Liu et al. [27] define the modified Young's modulus as

$$Y = \frac{1}{A_0} \frac{\partial^2 E}{\partial \epsilon^2} \bigg|_{\epsilon=0}. \quad (1.6)$$

Fig. 1.4 Strain energy and its first differential as a function of biaxial tensile strain [31]



This is the same definition as the in-plane stiffness [31]. They obtained $Y = 0.178 \text{ T Pa nm}$, about 40 % of the graphene value.

Qin et al. [31] showed that the anharmonic regime is reached for a biaxial strain in the range -2 to 4 % (Fig. 1.4), where the negative sign is for compressive strain. Beyond the harmonic regime, they identified two critical points. Beyond the first one ($\varepsilon_{c1} \approx 18$ % which they also call the “ultimate strain” [49]), $dE_s/d\varepsilon$ reaches a maximum value, i.e., it takes less tension to stretch the structure and it is unstable under certain acoustic waves (imaginary phonon frequencies), a phenomenon known as phonon instability. On the other hand, from an analysis of the phonon frequencies, Liu et al. determined that silicene would be unstable under a compressive biaxial strain larger than 5 %. Beyond the second critical point ($\varepsilon_{c2} \approx 20$ %), the strain energy decreases sharply and this corresponds to the yield point. Kaloni et al. [28] found this to occur for $\varepsilon \approx 17$ %. The change in the buckling parameter was reported by Kaloni et al. [28] and Peng et al. [47]. While an initial decrease with expansion is expected, both groups found the buckling to increase again for a strain larger than 10 %.

It has been pointed out that the strength of 2D materials can only be captured with hexagonal rings [47], leading to the need for a 6-atom unit cell for silicene. This unit cell allows one to model possible soft modes correctly. Most of the above calculations, though, have used smaller unit cells, which could be acceptable for smaller strains.

Mechanical response under a uniaxial strain has also been carried out [29, 30, 35, 47, 49]. Due to the difference in bond orientations, strain along perpendicular directions (conventionally taken to be x and y and chosen to be either the zigzag (ZZ) or armchair (AC) directions) could lead to different responses. For example, Qin et al. [49] found that the Poisson ratio is isotropic and constant for low strain (below 2 %) but then decreases (increases) for AC (ZZ) strain (Fig. 1.5a); similar results were obtained by Yang et al. [30]. Indeed, Wang et al. [29] obtained a Poisson ratio as high as 0.62 for ZZ strain. The response also becomes anisotropic beyond the harmonic regime (Fig. 1.5b). The ultimate strain was computed to be 0.17 (0.15) for AC (ZZ) strain. The buckling parameter, on the other hand, was

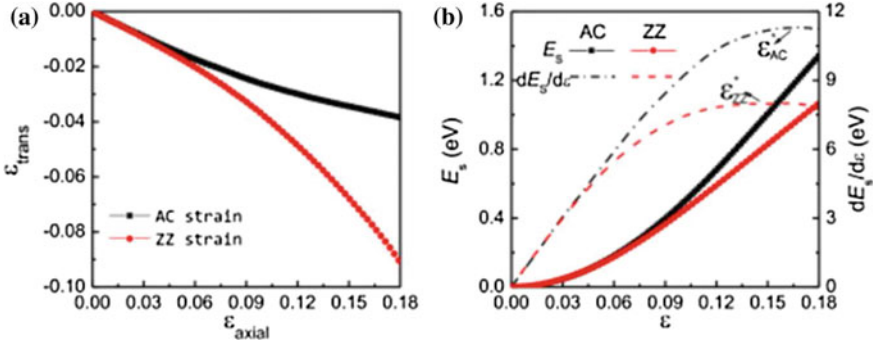


Fig. 1.5 **a** Transverse strain as a function of axial strain. **b** Strain energy and its derivative as a function of axial strain. From [49]

found to decrease in a linear fashion without chirality effects by Zhao [35], whereas Peng et al. [47] only found this result to be true until a strain of 0.16. Wang et al. [29] found the planar structure to be stable for a tensile strain of 0.2 while others found the buckling parameter to remain nonzero for uniaxial strains between -0.1 and 0.4 .

Zhao [35] defines the in-plane strength by

$$f_u = \sigma_u h, \quad (1.7)$$

where σ_u is the ultimate stress. She obtained f_u to be 5.66 N/m (ZZ) and 7.07 N/m (AC). Failure was identified for a tensile strain of 0.33 (ZZ) and 0.23 (AC). Yang et al. [30] used DFT-LDA to calculate the stress-strain relationships of low-buckled silicene. In addition to elastic instability, they also considered the possibility of phonon instability by computing the phonon frequencies; the latter was done using finite differences to compute the dynamical matrices for a $10 \times 10 \times 1$ supercell. Anharmonicity and anisotropy was found to set in for a strain larger than 0.03. The ideal strengths for equiaxial tension and AC uniaxial tension were found to be 7.59 N/m and 6.76 N/m, respectively. For ZZ uniaxial tension, there exists two ideal strengths (5.26 N/m and 5.29 N/m) due to the phase transition of silicene from the original low-buckled structure to a planar structure at a strain of 0.16. Phonon instability was found to occur after elastic instability. Instability for a biaxially strained structure at 0.22 strain occurred due to phonon modes perpendicular to the plane; this differs from graphene.

Classical MD (using the LAMMPS code) studies of the mechanical properties for large but finite nanosheets have been carried out [36, 50, 51]. Roman and Crawford [36] used a simulation region of 10×10 nm, the ReaxFF potential to describe Si-Si interactions, a microcanonical ensemble, and a nominal temperature of 10 K to limit temperature fluctuations but also to observe failure events. The obtained structural parameters were consistent with DFT values, though the buckling parameter was somewhat higher at 0.69 Å. The stress-strain curves

provide the Young's modulus (from the slope at small strain), tensile strength, and fracture strain (when the peak stress is reached). They also computed the out-of-plane bending stiffness by deforming the sheets into partial cylindrical tubes and minimizing the strain energy with respect to the curvature:

$$U = \frac{1}{2} D \kappa^2, \quad (1.8)$$

where κ , the curvature, was in the range of $0.05\text{--}0.3 \text{ nm}^{-1}$, and D is the bending modulus per unit width. D was obtained to be $38.63 \pm 0.501 \text{ eV}$. Silicene is more flexible but harder to break than silicon [51]. The fracture strength and strain were also found to be smaller at higher temperature; plasticity was not observed.

Summarizing the mechanical properties, the Young's modulus, bulk modulus and ultimate stress of silicene are predicted to be lower than for graphene. On the other hand, the Poisson ratio of silicene is higher than for graphene.

1.4 Electronic Properties

1.4.1 Band Structure

The silicene lattice is hexagonal leading to a hexagonal Brillouin zone. The unique band structure feature of silicene and graphene (in the absence of spin-orbit interaction) is the presence of valence and conduction bands with linear dispersions, so-called Dirac cones, crossing at the Fermi energy and at the K and K' points in the Brillouin zone. The Dirac cones form valleys in the Brillouin zone and the two degenerate bands at a given point originate from the A and B sublattices of the silicene structure. For graphene, these Dirac electrons originate from the p_z states on each sublattice; thus, in a tight-binding (TB) calculation, the Hamiltonian is of order 2 and the Dirac cones can be related to pseudospins. For silicene, due to the lack of mirror symmetry, p_z states are coupled to p_x and p_y states, as well as s states.

The band structure of buckled and flat silicene have been compared in a number of papers [1, 6, 19, 52] whereas Lebègue and Eriksson [23] compared silicene to planar Ge; similar calculations were performed by Houssa et al. [53–55], Wang [56] and Suzuki and Yokomizo [24]. Both forms of silicene have been shown to have electronic properties very similar to graphene [1, 6] in that they both have a zero $\pi\text{--}\pi^*$ gap at the K point. While the Dirac cones have been observed for graphene, it remains a prediction for free-standing silicene [1] and whether it is present for silicene on silver remains a controversy [57–65] in spite of early claims of observation [15, 66, 67].

All the above calculations were done by ignoring the spin-orbit coupling. Inclusion of the latter effect has shown that silicene would open a small gap of 1.55 meV and, therefore, might be better than graphene at displaying the quantum

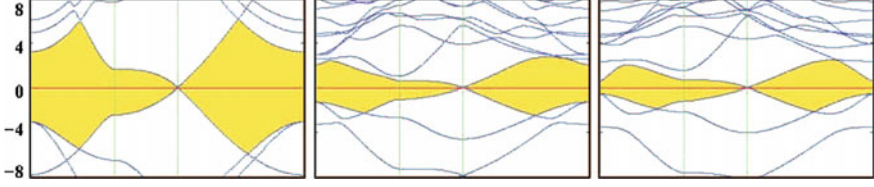


Fig. 1.6 DFT band structures of graphene, silicene and germanene. Reprinted figure with permission from [34]. Copyright (2009) by the American Physical Society

spin Hall effect (QSHE) [68]. The band structures of graphene, silicene and germanene, as obtained by Sahin et al. [34] are reproduced in Fig. 1.6.

While most calculations of the band structure have been carried out using ab initio methods, empirical methods such as TB [1, 68] and $k \cdot p$ [69, 70] have been used as well as they provide semi-analytical results, are much more efficient, and provide a physical picture. Beyond the linear approximation, the most general Hamiltonian for silicene allowed by symmetry can be written down as, to leading orders and in the presence of strain, electric field E and magnetic field B , (but without spin-orbit coupling) [70]

$$\mathcal{H} = \mathcal{H}_i + \mathcal{H}_e, \quad (1.9)$$

$$\mathcal{H}_e = \mathcal{H}^\epsilon + \mathcal{H}^E + \mathcal{H}^B, \quad (1.10)$$

$$\begin{aligned} \mathcal{H}_i = & a_1 (k_y \mathbf{J}_x - k_x \mathbf{J}_y) + a_2 (k_x^2 + k_y^2) \\ & + a_4 k_y (3k_x^2 - k_y^2) \mathbf{J}_z + a_5 (k_x^2 + k_y^2) (k_y \mathbf{J}_x - k_x \mathbf{J}_y) + \dots, \end{aligned} \quad (1.11)$$

$$\begin{aligned} \mathcal{H}^\epsilon = & e_1 (\epsilon_{xx} + \epsilon_{yy}) + e_2 \epsilon_{zz} + e_3 (\epsilon_{xx} + \epsilon_{yy}) (k_y \mathbf{J}_x - k_x \mathbf{J}_y) \\ & + e_4 [(\epsilon_{xx} - \epsilon_{yy}) k_y + 2\epsilon_{xy} k_x] \mathbf{J}_z + e_5 \epsilon_{zz} (k_y \mathbf{J}_x - k_x \mathbf{J}_y) + \dots, \end{aligned} \quad (1.12)$$

$$\begin{aligned} \mathcal{H}^E = & c_1 E_z \mathbf{J}_z + c_2 (E_x^2 + E_y^2) + c_3 E_z^2 + c_4 (E_x k_y - E_y k_x) \\ & + c_5 \left[(k_x^2 - k_y^2) E_x - 2k_x k_y E_y \right] + c_6 (E_x^2 + E_y^2) (k_y \mathbf{J}_x - k_x \mathbf{J}_y) \\ & + c_8 \left[(E_x^2 - E_y^2) k_y + 2E_x E_y k_x \right] \mathbf{J}_z + \dots, \end{aligned} \quad (1.13)$$

$$\mathcal{H}^B = b_1 (B_x \mathbf{J}_x + B_y \mathbf{J}_y) + b_2 B_z \mathbf{J}_z + b_3 (k_y B_x - k_x B_y) + \dots, \quad (1.14)$$

where the dots refer to higher-order terms. The a_i 's, b_i 's, c_i 's and e_i 's are $k \cdot p$ parameters. The $\mathcal{H}_i$ terms are intrinsic band-structure Hamiltonians while the other ones exist in the presence of external fields. In the above Hamiltonian, the $\mathbf{J}_i$ matrices represent the pseudospin degree of freedom and are the (2×2) Pauli spin matrices. In the band structure, the a_2 and a_3 terms provide quadratic in

k contributions while the a_4 and a_5 are of cubic order but only the a_4 term gives rise to an anisotropic term. Hence, one can readily see that the band structure of silicene to linear and quadratic orders is isotropic and anisotropic effects only manifest themselves if cubic terms become important. For comparison, the corresponding $\mathcal{H}$ for graphene [71] is

$$\mathcal{H} = a_{61}(k_y \mathbf{J}_x + k_x \mathbf{J}_y) + a_{11}(k_x^2 + k_y^2) + a_{62}[(k_y^2 - k_x^2) \mathbf{J}_x + 2k_x k_y \mathbf{J}_y], \quad (1.15)$$

and the anisotropic term is quadratic in the wave vector.

In the presence of spin-orbit coupling, Ezawa [72] gave

$$H_\eta = \hbar v_F(\eta k_x \tau_x + k_y \tau_y) + \lambda_{\text{SO}} \eta \tau_z \sigma_z + a \lambda_{R2} \eta \tau_z (k_y \sigma_x - k_x \sigma_y), \quad (1.16)$$

where $\eta = \pm 1$ for the two valleys K and K' , σ_z are the Pauli matrices associated with the electron spin, τ_z are the Pauli matrices associated with pseudospin, and the Rashba term is now present due to inversion asymmetry.

The Fermi velocity of the linear bands is an important parameter. Using DFT, Cahangirov et al. [19] estimated them to be $\sim 10^6$ m/s for silicene, basically the same value as for graphene. However, Guzmán-Verri and Lew Yan Voon [1], using TB models, evaluated them to be $\sim 10^5$ m/s for silicene. Dzade et al. [48] also obtained a smaller Fermi velocity for silicene. More recent calculations also find a slightly smaller value for silicene than for graphene. This can be easily understood from the reduced hopping in silicene since the Si atoms are more distant from each other.

1.4.2 Strain

A few calculations of a free-standing silicene sheet under strain have been carried out [27–31, 35, 49, 73–76]. The standard approach is to first obtain the unstrained relaxed structure and then distort the unit cell in the appropriate direction such that the strain in that direction is given by

$$\epsilon = \frac{a - a_0}{a_0}, \quad (1.17)$$

where a_0 (a) is the equilibrium (strained) lattice parameter. Since the symmetry is reduced for a uniaxial strain, it is convenient to use a rectangular 1×2 supercell with four atoms. However, a larger unit cell is needed in order to correctly simulate the strength of the nanosheet [47].

A relatively large strain can be applied to the nanosheets and a biaxial strain is a natural expectation if the sheets are deposited on a substrate. A biaxial tensile strain was found to lead to a semimetal-metal transition when the strain is larger than 7 % [27, 28, 31, 73]. This is due to the lowering of the conduction band at the Γ -point;

the Dirac point was also found to increase in energy (but remaining degenerate) [31], leading to the possibility of *p*-type self-doping [28]. Similarly, biaxial compressive strain leads to a lowering of the Dirac point below the Fermi level, leading to *n*-type doping [73]. These changes have been correlated with the changing character of the bonding between sp^3 and sp^2 . The above change in character does not occur for graphene since the bonding is pure sp^2 and the atoms remain in a plane. The Fermi velocity is found to decrease slowly with strain, decreasing to 94 % of the unstrained value for strain up to 7 % [31]. Biaxial strain is also found to lead to superconductivity [74]. In particular, for an electron doping of $3.5 \times 10^{14} \text{ cm}^{-2}$ and a tension of 5 %, the critical temperature was calculated to be 18.7 K using the Eliashberg theory.

On the other hand, a uniaxial strain is expected to lead to a gap opening due to the symmetry lowering. Indeed, a gap was reported to open up for uniaxial tensile strain, up to 0.08 eV for strain along the zigzag (ZZ) direction and up to 0.04 eV for strain along the armchair (AC) direction [35], at about 8 and 5 %, respectively (Fig 1.7). Mohan et al. [75] similarly obtained a small band gap for tensile strain but found that a direct band gap of 389 meV is formed for 6 % uniaxial compression. An indirect band gap of 379 meV is found for 6 % biaxial compression. They computed the corresponding deformation potentials,

$$\frac{dE}{d\epsilon}, \quad (1.18)$$

and found them to be fairly constant for strains below around 6 %. However, Qin et al. [49] and Yang et al. [30] did not obtain a gap and only obtained the Dirac point to shift. The latter interpreted the disagreement of Zhao to the latter not using sufficient k points near the crossing. The lack of band-gap opening has been confirmed using $k \cdot p$ theory [70]; from (1.12), it can be seen that both bands at the Dirac point have the same deformation potential, which means they would both be affected equally by the strain. Qin et al. did obtain a dependence of the Fermi velocity with the type of uniaxial strain as well as a wave-vector dependence. Yang et al. also included spin-orbit coupling in their calculations. The spin-orbit coupling

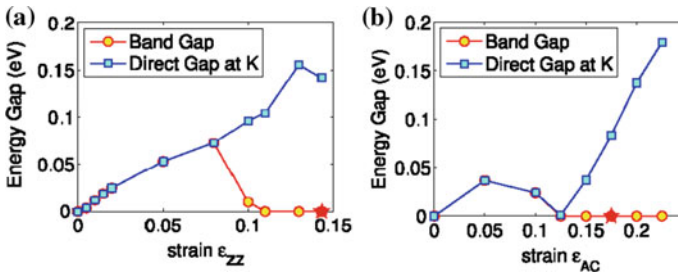


Fig. 1.7 DFT-PBE band gap with uniaxial tensile strain for silicene. Reprinted from [35]. Copyright (2012), with permission from Elsevier [35]

gap was found to initially decrease with increasing strain and then increase again after a strain of about 0.05.

Qin et al. computed the work function as a function of strain. The work function is defined as the minimum energy to remove an electron and is given by

$$\Phi = E_{\text{vac}} - E_F. \quad (1.19)$$

The vacuum energy E_{vac} was determined as the average electrostatic potential energy in a plane parallel to the silicene layer and asymptotically away. For a biaxial strain, the work function initially increased from the unstrained value of 4.8 eV, then saturates to around 5.1 eV for a strain above 15 % [31]. For a uniaxial strain [49], the change is isotropic up to 3 % beyond which the ZZ strain leads to a larger work function but no saturation is observed. The strain dependence has been interpreted in terms of the change in the Fermi level.

1.5 Electric Field

Electric field effects on silicene have been investigated [77–79]. The field has an effect on the buckling parameter. The vertical electric field was found to increase the buckling parameter quadratically with the field [77].

Ni et al. [77] found that a vertical electric field opened a band gap in single layer silicene, contrary to graphene, and the gap increased linearly with the field up to about 1 V/Å. The reason for the gap opening is because the two atoms in the unit cell experience different electric potentials due to the different heights. Geometry optimization and electronic structure was performed using Dmol³. Ni et al. obtained a rate of 0.157 eÅ while Drummond et al. [78] got 0.0742 eÅ. The latter also indicated that the gap actually starts closing for $E_{\perp} \approx 0.5 \text{ VÅ}^{-1}$ due to the overlap of the conduction band at Γ and the valence band at K . The electric field also leads to an almost linear increase in the effective mass; for example, for a field of 0.4 V/Å, the hole mass was found to be $0.015m_0$ ($0.033m_0$) along the $K\Gamma$ (MK) direction and about 2 % different for the electron mass.

1.6 Topological Properties

Silicene is similar to graphene in being a Kane-Mele type 2D topological insulator (TI) [80]. A TI has a bulk energy gap but gapless edge states that allow correlated charge and spin transport (Fig. 1.8). They can be distinguished from the more common band insulators because the charge transport is protected from disorder (due to the correlation with spin) and, mathematically, this can be represented by a different topological order or quantum number, the Z_2 invariant [82]. There are two topological quantum numbers: the Chern number C and the Z_2 index. The latter is

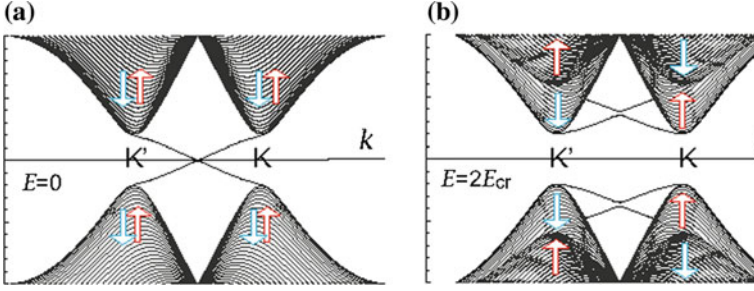


Fig. 1.8 One-dimensional energy bands for a silicene nanoribbon. **a** The bands crossing the gap represent edge states, demonstrating that it is a topological insulator. **b** All states are gapped, demonstrating that it is a band insulator. Reproduced from [81] with kind permission from Springer Science and Business Media

also the same as the spin-Chern number C_s when the spin σ_z is a good quantum number. Qualitatively, this is so far no different from graphene. Indeed, Liu et al. [68] used the fact that the Hamiltonian of the buckled structure can be continuously obtained from the flat one [1] to demonstrate the QSH state for silicene. The QSH of the TI is generated with the assistance of the spin-orbit coupling. The larger spin-orbit coupling gap of 1.55 meV [68] for silicene makes it more practical than graphene for realizing a TI.

It can be expected that the topological properties for silicene would be different from graphene in the presence of an external electric field since the buckled structure of silicene leads to a gap opening, contrary to the case for graphene. In fact, the interplay of the spin-orbit gap and an electric field induced gap allows for a transition between a TI and a band insulator (where the gapless edge states are not protected by topology). This quantum phase transition was computed to occur for a vertical field of 20 mV/Å [78]. Additionally, this is accompanied by a transition from the QSHE to the quantum valley Hall effect (QVHE) [83, 84]. In the presence of an exchange field M and an electric field E_z , one can plot a phase diagram (Fig. 1.9). Ezawa computed four principal phases [81]: band insulator (BI), quantum anomalous Hall (QAH), quantum spin Hall (QSH), valley-polarized metal (VPM) and spin valley-polarized metal (SVPM). The QAH is characterized by an insulating bulk gap and chiral gapless edges; it is induced by the internal magnetization and by the spin-orbit coupling, i.e., it displays quantized Hall conductance in the absence of an external magnetic field. The valley-polarized metal refers to silicene with electrons moved from the conduction band at K to the valence band at K' in a perpendicular electric field. Ezawa has further exploited the buckled structure of silicene to postulate additional topological phases not encountered for graphene. Thus, an inhomogeneous electric field is shown to generate a helical zero mode away from the edges by closing the band gap spatially [85], while circularly polarized light was used to trigger a topological phase transition from one TI to another TI as a result of the photon dressing of the bands [86]. It was also postulated to break the valley degeneracy by introducing different exchange fields on

Thus, a B-substituted silicene structure with the stoichiometry B:Si = 1:3 has been considered [103] or a study of Ni-doping was done with a stoichiometry of 1:2 [104]. In this section, we restrict ourselves to the few studies of low doping on the electronic properties [105]. Possibly the only study of low doping on silicene looked at the change in the Fermi energy and in the structure [105]. They found the DFT calculations to follow fairly well the analytical relation resulting from a linear energy dispersion:

$$\sigma = \text{sign}(E_F) \frac{E_F^2}{(\text{eV})^2} C \times 10^{13} \text{ cm}^{-2}, \quad (1.20)$$

where σ is the charge carrier concentration and E_F the Fermi energy. Any deviation between the DFT points and the analytical curve was attributed to the deviation of the band structure from the ideal linearity. The lattice was also found to expand (shrink) when electrons are added (removed); the latter result is similar to graphene [105].

1.8 Optical Properties

A fascinating property of graphene is the universal low-frequency optical absorbance predicted by a non-interacting Dirac fermion theory in 2D and equal to $\pi\alpha$, where $\alpha = 1/137.076$ is the Sommerfeld fine structure constant; this has been observed experimentally [106]. Since this result is independent of the atomic species, buckling, and orbital hybridization, it should apply to silicene as well. A proof based upon the independent-particle approximation has been provided [107].

Optical properties have been computed using DFT [107–111]. Figure 1.10 compares the results for graphene, silicene and germanene obtained in the absence

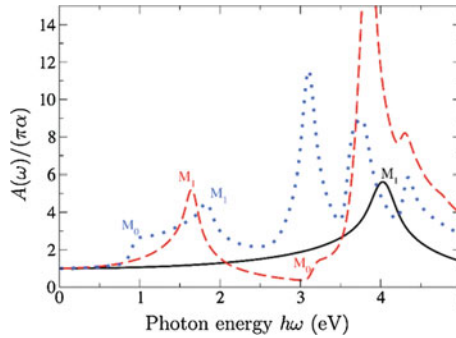


Fig. 1.10 Spectral absorbance of graphene (black solid line), silicene (red dashed line) and germanene (red dotted line). Reprinted figure with permission from [108]. Copyright (2013) by the American Physical Society

of self-energy and excitonic corrections and at normal incidence. The optical properties at higher energies do differ due to differences in the band structure. Inclusion of quasiparticle many-body effects was found to have no influence on the low-frequency absorbance but led to a blueshift of the peaks at higher energies, mainly because of the increase in the interband energies [109]. However, inclusion of spin-orbit coupling leads to important changes at low frequency [109]. First, a SO gap is opened leading to transparency. Second, the near-gap absorbance is enhanced by a factor of 2; this is due to the fact that we now have the equivalent of a massive Dirac particle in 2D. Third, the absorbance decays back down to the universal value between the gap and the higher-energy peaks.

The dielectric functions also reveal the nature of the plasmons (collective excitations of the electron gas) since the latter are probed using electron energy loss spectroscopy (EELS) and peaks in the latter correspond to dips in the imaginary part of the dielectric function, $\epsilon_2(\omega)$. Two features in EELS of silicene for in-plane polarization are below 5 eV and above 5 eV, corresponding to the π and $\pi + \sigma$ peaks, respectively. The π plasmon results from the collective $\pi-\pi^*$ transitions while $\pi + \sigma$ plasmon results from the $\pi-\sigma^*$ and $\sigma-\sigma^*$ transitions [112]. The energies are lower than for graphene [110]. Calculations of the dielectric properties [75] show that the π plasmon in silicene disappears with tensile and asymmetric strains; the $\pi + \sigma$ plasmons are red-shifted for tensile strains; and the $\pi + \sigma$ plasmons are blue-shifted for compressive strains. Plasmons have been proposed as probes of topological phase transitions [113, 114].

Temperature effects on plasmons have been studied [115]. At $T = 0$ and in the absence of the spin-orbit gap, only interband transitions are possible. At finite temperature, intraband transitions become possible as well. The low density-of-state (DOS) at the Dirac point reduces the likelihood of low-frequency plasmons. However, the SO gap for silicene increases the DOS and, at finite temperatures, allows intraband plasmons as well as interband ones. When the zero of ϵ_1 is in the gap of ϵ_2 , the plasmon is undamped. At a critical temperature, the interband transition is negligible and the intraband one dominates, leading to damped plasmons.

The effect of aluminium (Al) and phosphorus (P) substitutional doping on the optical properties has been studied [116] and found to differ from graphene. For EELS with parallel polarization, similar to the results for graphene, no new EELS peak occurs. However, for perpendicular polarization, two new EELS peaks emerge for P doping and was attributed to the buckling in silicene.

1.9 Transport

Charge carrier transport is one of the motivations for studying silicene given the potential for transistor action and compatibility with current Si electronics. While the carrier mobility in silicene will be strongly dependent upon the environment it is in, understanding the intrinsic mobility for a free-standing film is still important. A recent calculation [37] obtained an electron (a hole) mobility of

$2.57 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ($2.22 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) at room temperature, slightly lower than for graphene but much larger than for bulk Si. They used a deformation potential theory and the Boltzmann transport equation, with acoustic phonons as the scattering source. The deformation potential was calculated by stretching and compressing the lattice by up to 1.5 % along the zigzag and armchair directions. A kinetic equation approach within the relaxation time approximation, treating a finite-temperature screened electron-impurity interaction, has been used to investigate transport in the presence of impurities and a gap [117]. A residual conductivity is found when the chemical potential is in the gap and arises from interband correlation.

1.10 Magnetic Properties

We here consider the effect of an external magnetic field on the electronic properties. For standard semiconductors, this is typically observed by performing a magneto-optical experiment, whereby the Landau levels formed are probed by optical transitions. This is a very sensitive approach to characterizing the band structure. For free-standing silicene, magneto-optical properties have been studied theoretically revealing interesting spin-valley effects [118–121]. For example, the low-energy dispersion is obtained from (1.16) with the neglect of the Rashba SO term as

$$E_n = \text{sgn}(n) \sqrt{\frac{1}{4} \Delta_{\text{SO}}^2 + 2|n|v_F^2 \hbar e B}, \quad (1.21)$$

for $n \neq 0$ and $E_n = \sigma \eta \Delta_{\text{SO}}/2$ for $n = 0$, where n is the subband index, and when starting with the Dirac-Kane-Mele Hamiltonian (Fig. 1.11). The selection rules for interband transitions are found to be $\Delta n = \pm 1$.

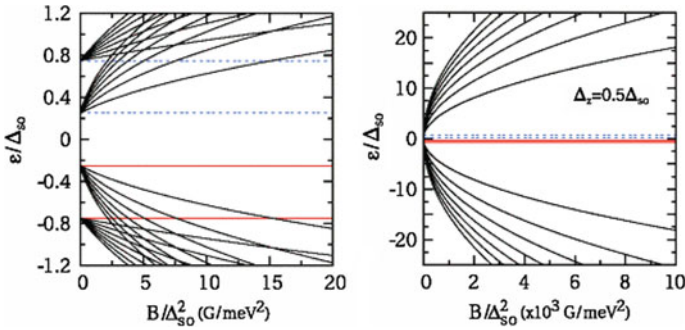


Fig. 1.11 Landau levels as a function of magnetic field for small (*left*) and large (*right*) field. Reprinted figure with permission from [119]. Copyright (2013) by the American Physical Society

For graphene, Chang [122], using a simple effective-mass approach and the Luttinger-Kohn formalism [123], showed that the Landau levels are given by

$$E_n = \text{sgn}(n)\sqrt{2}\hbar v_F \sqrt{|n|B}. \quad (1.22)$$

The basic result is that the positions and intensities of the absorption lines scale with $\sqrt{B}$ and that the line corresponding to the transition from the lowest $n = 0$ to the $n = 1$ Landau level is anomalous due to the Dirac nature [124]. This behaviour has been observed in infrared spectroscopy [125–127].

The effect on the band structure in the presence of an external electric field and a perpendicular magnetic field has also been studied [128]. They found that, for finite E_z , the spin and valley degeneracies of the Landau levels are lifted and this leads to additional plateaus in the Hall conductivity, at half-integer values of $4e^2/h$, due to spin intra-Landau-level transitions that are absent in graphene.

1.11 Phonons

A number of papers have included a calculation of phonon modes in order to establish the stability of structures obtained by energy minimization [19, 28, 48]. The dispersion relations for graphene and silicene are compared in Fig. 1.12. The highest G- and D-modes are 550 and 545 cm^{-1} [28].

Silicene has a flexural mode, as does graphene. However, because of the symmetry reduction due to the buckling, this mode for silicene has both a z and an xy component [41].

Dzade et al. [48] reported significant violation of the acoustic sum rule when using density functional perturbation theory within the Born-Oppenheimer approximation; hence, they reported results using the frozen phonon method. They found the flexural modes to be much smaller in energy than for graphene leading to the conclusion that silicene would more likely form ripples.

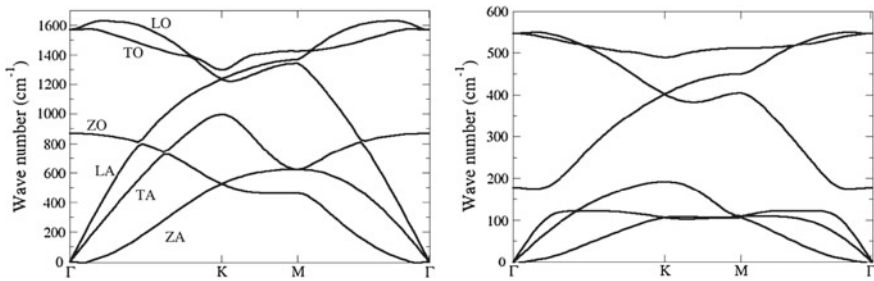


Fig. 1.12 Phonon spectrum for graphene (*left*) and silicene (*right*). Reprinted from [155], Copyright (2014), with permission from Elsevier

Kaloni et al. [28] studied the change in the phonon spectrum under tensile biaxial strain. All the modes soften with increasing strain due to the weakening of the Si–Si bond. They obtained negative frequency modes for a strain larger than 17 %. They also computed the Grüneisen parameter for the G-mode:

$$\gamma_G = -\frac{\Delta\omega_G}{2\omega_G^0\epsilon}, \quad (1.23)$$

where ω_G^0 is the unstrained frequency and $\Delta\omega_G$ is the change in the frequency under the biaxial strain. The Grüneisen parameter was found to decrease from 1.64 ($\epsilon = 5\%$) to 1.34 ($\epsilon = 20\%$) and then increase again, following the trend with the buckling parameter.

Electron-optical phonon coupling matrix elements are calculated to be small [129], being about a factor of 25 times smaller than in graphene. A consequence is that long momentum relaxation lengths and high carrier mobilities are predicted for silicene as carrier relaxation via phonon scattering is inhibited.

1.12 Thermal Properties

A few thermal properties have been studied.

1.12.1 Thermal Stability

The thermal stability has been studied using reactive MD [130] and pristine silicene was found to be stable up to 1500 K, after which it formed a three-dimensional amorphous structure. Defects have been found to reduce the thermal stability of silicene by as much as 30 % [130]. Passivating the defects improves the stability.

1.12.2 Lattice Thermal Conductivity

As a semimetal, the thermal conductivity of silicene has been assumed to be mainly due to phonon transport. Initial calculations have used classical MD and gave values in the range 5–65 W/mK at 300 K. Thus, an equilibrium MD simulation using Tersoff bond-order potential and the Green-Kubo approach for κ on a variety of supercells ranging from 5×3 to 17×10 gave an in-plane thermal conductivity κ of 20 W/mK [131], compared to a value of ~ 3000 – 5000 W/mK for suspended graphene [42] and 150–200 W/mK for silicon. It should be noted that they observed a small anisotropy in the value of the conductivity of the order of 1–4 W/mK and a general trend of increasing κ with increasing supercell size. From an analysis of the

partial density of states (PDOS), they associated the reduction in κ to two reasons. One is the lowering of the PDOS for frequencies below 20 THz (phonon softening), and the other is due to the blueshift in the PDOS to higher frequencies (phonon stiffening). The result is a reduction in the phonon modes present for heat conduction at low temperatures.

Nonequilibrium MD simulations have also been carried out [132–137]. Wang and Sun, Hu et al., Ng et al., Liu et al. (who also used the Stillinger-Weber potential), and Yeo and Liu used the Tersoff potential, while Pei et al. used the MEAM potential. Hu et al. used a simulation region with 1000 unit cells in one direction and the atomic positions were relaxed. Thermal conductivity was then calculated using non-equilibrium MD and extracted from the Fourier law by computing the heat flux [133]. They found that κ (~ 40 W/mK) is significantly influenced by the out-of-plane flexural modes. However, studies have shown that the Tersoff potential for bulk Si does not reproduce the buckling [133]; the MEAM potential used by the latter gave a buckling of 0.85 nm at 10 K, which is doubled accepted values. This work (as well as Wang and Sun) also used the reverse non-equilibrium MD whereby the heat flux is imposed and the temperature gradient obtained; there is a length dependence to κ and they studied in the range of 33–210 nm. They got a similar κ to the work by Pei et al. [134]. On the other hand, Wang and Sun (Ng et al.) got a κ of about 55(65) W/mK and Liu et al. [136] got 55–65 W/mK. Studies as a function of length have also been carried out using MD [137]. Graphene was found to possess significantly higher thermal conductivities than silicene at every length scale and chirality, and this was attributed to the higher phonon group velocities of the dominant acoustic modes in graphene.

Zhang et al. [138] has used a modified Stillinger-Weber potential in their study and the LAMMPS code. They were able to reproduce the buckling of silicene and phonon dispersions in agreement with DFT. In their case, they did both equilibrium and non-equilibrium MD as well as using anharmonic lattice dynamics (ALD). The MD methods gave a κ below 12 W/mK while the ALD results could be even lower. They used the ALD method to obtain the phonon mode contributions. They deduced that more than 50 % of the thermal conductivity is due to phonon modes with wavelengths less than 10 nm. Their conclusion, though, differs from the other work cited above. They deduced that as much as 80 % of κ arises from in-plane longitudinal modes, with most of the rest due to the transverse modes. Another calculation using the Tersoff potential instead also found the in-plane phonons to contribute over 85 % to κ . Nevertheless, they also associate the difference to phonon softening and phonon stiffening.

The temperature dependence of the thermal conductivity of free-standing and SiO₂ supported silicene has been investigated using both equilibrium and non-equilibrium MD from 300 to 900 K [139], inclusive of quantum corrections. The substrate leads to a 78 % reduction at 300 K. However, Zhang et al. [140] found that the thermal conductivity could either increase or decrease depending on the substrate. Thus, they found an increase in the thermal conductivity of silicene supported on the 6H-SiC substrate and attributed this increase to the augmented lifetime of the majority of the acoustic phonons, while they found a significant

decrease in the thermal conductivity of silicene supported on the 3C-SiC substrate results, due to the reduction in the lifetime of almost the entire phonon spectrum. This is in contrast to graphene where substrates have been found to always lead to a decrease in the phonon transport [140]. For suspended silicene, κ has been computed over $0 < T < 400$ K [141]. They obtained a maximum value of about 100 W/mK near 100 K, compared to around 1000 W/mK for bulk Si [141] and 3000–5000 W/mK for graphene.

Xie et al. [41] reported a value of 9.4 W/mK at 300 K using first-principles calculations; out-of-plane vibrations was only found to contribute less than 10 % of the overall thermal conductivity. The difference compared to graphene was related to the buckling which breaks the reflection symmetry and leads to scattering of the flexural modes with other modes as the former are no longer pure out-of-plane vibrations.

The effect of defects [131], strain [133, 134], and isotopic doping [134, 136] on κ has been studied. Not surprisingly, defects were found to reduce κ due to the increased defect-phonon scattering. In fact, Li and Zhang [131] found that removing a single atom out of 448 atoms from the domain led to a 78 % reduction in κ . Under tensile strain, κ was found to initially increase at small strains (below 4 %) and then decrease with larger strains [134]; this was done on a $33 \text{ nm} \times 33 \text{ nm}$ silicene sheet. The initial increase could be attributed to the reduced buckling under strain and, therefore, an increase in in-plane stiffness. Higher strains lead to stretching of the Si–Si bonds and, therefore, a decrease in in-plane stiffness. Isotopic doping is found to decrease κ as well; for example, 50 % of ^{30}Si in a ^{28}Si lattice led to a 20 % reduction.

Thermal conductance G and rectification at an interface with graphene has been studied [142]. They found that G not only increases with the temperature but also with the monolayer length at a given temperature until it reaches a saturated value. At 300 K, the saturated value is $250 \text{ MW/m}^2 \text{ K}$. In contrast, they found that R decreased with increasing monolayer length and temperature. Both G and R were significantly affected by tensile strain applied on silicene along the interface direction, but both were almost independent of the heat flux J . They determined a critical value $J = 42 \text{ GW/m}^2$ above which low-frequency kinetic waves were excited and provided an additional channel for heat transport.

1.12.3 Thermopower and Thermoelectricity

The lower thermal conductivity of silicene compared to graphene could be advantageous for thermoelectric properties since the latter are improved by lower thermal conductivity and higher thermopower. Thermopower is defined by the

voltage drop that appears across a material due to an imposed temperature gradient, and a measure is via the Seebeck coefficient,

$$S = \frac{1}{eT} \frac{L_1}{L_0}, \quad (1.24)$$

where T is the temperature and

$$L_m(\mu) = \frac{2}{h} \int_{-\infty}^{\infty} dE T(E) (E - \mu)^m \left(-\frac{\partial f(E, \mu)}{\partial E} \right), \quad (1.25)$$

where $T(E)$ is the transmission at energy E , $F(E, \mu)$ is the Fermi-Dirac distribution, and μ is the chemical potential. The thermopower was calculated with and without an external field [43]. A four-band TB model was used for the electronic band structure, transport properties were calculated using the non-equilibrium Green's function method, and the simulation length was 1000 unit cells. They found the thermopower to be somewhat insensitive to temperature changes between 100 and 500 K and to have a peak value of 87 $\mu\text{V/K}$. In the presence of an electric field, and with the chemical potential in the band gap, there is an increase in κ up to 300 $\mu\text{V/K}$ at 300 K.

Thermoelectricity is measured by the figure of merit,

$$ZT = \frac{\sigma S^2 T}{\kappa}, \quad (1.26)$$

where σ is the electrical conductance. The thermoelectric coefficients of silicene at room temperature have been computed [45] using the BOLTZTRAP and VASP codes. They were found to have a ZT_c less than 0.5. On the other hand, for graphene, the figure of merit has been estimated to be 0.17–1.02 for isotope-doped graphene with a sheet carrier concentration of 10^{16} – 10^{17} m^{-2} and a temperature of 300–450 K [46].

1.13 Stability to Oxidation

A DFT study of the stability to oxygen exposure has been carried out [143, 144]. They found that the molecule dissociates easily on silicene without any energy barrier and the oxygen atoms form strong bonds with Si atoms. Coupled with the low diffusivity, oxides are formed. Hence, silicene is predicted to be unstable in air. In a subsequent work, they have also studied the stability of silicane [144]. There are now two minor energy barriers of O_2 molecule adsorption and dissociation on silicane, thus silicane has higher stability than free-standing silicene in oxygen. However, they also argue that, once the O_2 molecule dissociates into two O atoms,

desorption of O atoms will be very difficult due to its high energy barrier. An experimental study of oxidation showed the availability to create a band gap [145].

1.14 Defects

Given that defects are always present in real samples, it is useful to briefly discuss the variety of defects than can exist in silicene and the impact on certain physical properties.

The simplest type of defect would be a point defect such as a vacancy [146, 147]. For graphene, the ground state is a nonmagnetic reconstructed monovacancy (MV) [147]. For silicene, on the other hand, the three Si atoms around the symmetric MV core move to the core center and eliminate their dangling bonds by forming a fourth bond, becoming nonmagnetic [146]. However, this has subsequently been found not to be the lowest energy MV. A vacancy type, monovacancy MV-1, not previously found in graphene, has been predicted in silicene using first-principles calculations [147] on a 8×8 unit cell. It has a planelike sp^3 hybridization at its defect core. The diffusion coefficient of MV-1 is calculated to be $2.3 \times 10 \text{ cm}^2/\text{s}$, much higher than that of the MV in graphene. Silicene with MV-1 is metallic.

Vacancy clusters, extended line defects (ELDs), and adatoms have been studied using first-principles calculations [148, 149]. Divacancies have been found to have lower mobilities than single vacancies [148] and divacancies induce small gaps in silicene. Si adatoms induce long-range spin polarization and a band gap, thus achieving an all-silicon magnetic semiconductor. Small defects were found to have a tendency to coalesce forming highly stable vacancy clusters [149]. The 5|8|5 ELD was found to be easier to form in the silicene than graphene because of the mixed sp^2/sp^3 hybridization of silicene. Stone-Wales defects have also been studied [148, 150, 151]. The Stone-Wales defect is a topological defect formed by the 90° rotation of a dimer bond which results in four hexagons turning into two pairs of pentagon-heptagon rings (Fig. 1.13). In particular, it was found that the

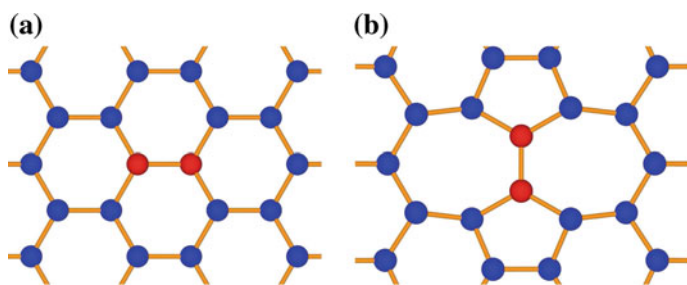


Fig. 1.13 Representation of a Stone-Wales defect in silicene. Reprinted from [150], Copyright (2014), with permission from Elsevier

formation energy and kinetic barrier are lower in silicene than in graphene. A band gap of 0.01 eV is created. The effect of vacancies and Stone-Wales defects on the mechanical properties have been studied using molecular dynamic finite element method with Tersoff potential [152]. They found that pristine and lowly defective silicene sheets exhibit almost the same elastic nature up to the fracture points. However, a single defect significantly weakened the silicene sheet, leading to a considerable reduction in the fracture strength. Thus, one 2-atom vacancy in the reduced the fracture stress by 1820 % and the fracture strain by 3335 %. The weakening effects of Stone-Wales defects varied with the tensile direction and the orientation of these defects.

A defect that is particular to 2D materials but absent for graphene is the buckling interface formed between two pieces of silicene with oppositely oriented buckling [153]. This leads to a line defect that has a low formation energy but has a higher reactivity than the pristine silicene itself. The latter was deduced by studying the adsorption of a single gold atom and they turn out to have a binding energy of -3.50 eV.

1.15 Summary

Silicene is another example of the novel materials belonging to the class of 2D materials beyond graphene. Yet, it has some differences since the sheet is puckered, has a different point-group symmetry and a different pseudospin. Thus, it is predicted to have Dirac cones just as for graphene but with a larger spin-orbit gap and with a band gap opening under a perpendicular electric field. Physical properties are, generally, less extreme than for graphene (e.g., slightly lower mechanical strengths and electron Fermi velocity) but it can also have “better” physical properties such as better thermoelectric figure of merit and a richer topological phase diagram.

Currently, free-standing silicene (without functional groups) have not been realized experimentally. Nevertheless, a proper understanding of the properties of free-standing silicene is a good starting point for understanding the properties of silicene on a substrate or of functionalization.

References

1. G.G. Guzmán-Verri, L.C. Lew Yan Voon, Phys. Rev. B (Condens. Matter Mater. Phys.) **76** (7), 075131 (2007). doi:[10.1103/PhysRevB.76.075131](https://doi.org/10.1103/PhysRevB.76.075131). URL <http://link.aps.org/abstract/PRB/v76/e075131>
2. K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Science **306**(5696), 666 (2004)
3. K. Takeda, K. Shiraishi, Phys. Rev. B **39**(15), 11028 (1989). doi:[10.1103/PhysRevB.39.11028](https://doi.org/10.1103/PhysRevB.39.11028)

4. K. Takeda, K. Shiraishi, *Phys. Rev. B* **50**(20), 14916 (1994). doi:[10.1103/PhysRevB.50.14916](https://doi.org/10.1103/PhysRevB.50.14916)
5. Y. Wang, K. Scheerschmidt, U. Gösele, *Phys. Rev. B* **61**, 12864 (2000). doi:[10.1103/PhysRevB.61.12864](https://doi.org/10.1103/PhysRevB.61.12864). URL <http://link.aps.org/doi/10.1103/PhysRevB.61.12864>
6. X. Yang, J. Ni, *Phys. Rev. B* **72**(19), 195426 (2005). doi:[10.1103/PhysRevB.72.195426](https://doi.org/10.1103/PhysRevB.72.195426)
7. E. Durgun, S. Tongay, S. Ciraci, *Phys. Rev. B* **72**(7), 075420 (2005)
8. H. Nakano, M. Ishii, H. Nakamura, *Chem. Commun.* 2945–2947 (2005). doi:[10.1039/B500758E](https://doi.org/10.1039/B500758E). URL <http://dx.doi.org/10.1039/B500758E>
9. H. Nakano, T. Mitsuoka, M. Harada, K. Horibuchi, H. Nozaki, N. Takahashi, T. Nonaka, Y. Seno, H. Nakamura, *Angew. Chem.* **118**(38), 6451 (2006)
10. A. Kara, C. Léandri, M.E. Dávila, P. de Padova, B. Ealet, H. Oughaddou, B. Aufray, G.L. Lay, *J. Supercond. Novel Magn.* **22**, 259 (2009)
11. D. Chiappe, C. Grazianetti, G. Tallarida, M. Fanciulli, A. Molle, *Adv. Mat.* **24**, 5088 (2012)
12. B. Feng, Z. Ding, S. Meng, Y. Yao, X. He, P. Cheng, L. Chen, K. Wu, *Nano Lett.* **12**(7), 3507 (2012). doi:[10.1021/nl301047g](https://doi.org/10.1021/nl301047g). URL <http://pubs.acs.org/doi/abs/10.1021/nl301047g>
13. H. Jamgotchian, Y. Colignon, N. Hamzaoui, B. Ealet, J.Y. Hoarau, B. Aufray, J.P. Bibérian, *J. Phys. Condensed Mat.* **24**(17), 172001 (2012)
14. C.L. Lin, R. Arafune, K. Kawahara, N. Tsukahara, E. Minamitani, Y. Kim, N. Takagi, M. Kawai, *Appl. Phys. Express* **5**, 045802 (2012)
15. P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M.C. Asensio, A. Resta, B. Ealet, G. Le Lay, *Phys. Rev. Lett.* **108**, 155501 (2012). Doi:[10.1103/PhysRevLett.108.155501](https://doi.org/10.1103/PhysRevLett.108.155501). URL <http://link.aps.org/doi/10.1103/PhysRevLett.108.155501>
16. L. Tao, E. Cinquanta, D. Chiappe, C. Grazianetti, M. Fanciulli, M. Dubey, A. Molle, D. Akinwande, *Nat. Nano.* **10**, 227 (2015)
17. J.R. Soto, B. Molina, J.J. Castro, *Phys. Chem. Chem. Phys.* **17**, 7624 (2015). doi:[10.1039/C4CP05912C](https://doi.org/10.1039/C4CP05912C). URL <http://dx.doi.org/10.1039/C4CP05912C>
18. Y. Ding, J. Ni, *Appl. Phys. Lett.* **95**(8), 083115 (2009)
19. S. Cahangirov, M. Topsakal, E. Aktürk, H. Sahin, S. Ciraci, *Phys. Rev. Lett.* **102**(23), 236804 (2009)
20. L.C. Lew Yan Voon, E. Sandberg, R.S. Aga, A.A. Farajian, *Appl. Phys. Lett.* **97**, 163114 (2010)
21. D. Kaltsas, L. Tsetseris, *Phys. Chem. Chem. Phys.* **15**(24), 9710 (2013). doi:[10.1039/C3CP50944C](https://doi.org/10.1039/C3CP50944C). URL <http://dx.doi.org/10.1039/C3CP50944C>
22. M.T. Yin, M.L. Cohen, *Phys. Rev. B* **29**, 6996 (1984). doi:[10.1103/PhysRevB.29.6996](https://doi.org/10.1103/PhysRevB.29.6996). URL <http://link.aps.org/doi/10.1103/PhysRevB.29.6996>
23. S. Lebegue, O. Eriksson, *Phys. Rev. B (Condens. Matter Mater. Phys.)* **79**(11), 115409 (2009). doi:[10.1103/PhysRevB.79.115409](https://doi.org/10.1103/PhysRevB.79.115409). URL <http://link.aps.org/abstract/PRB/v79/e115409>
24. T. Suzuki, Y. Yokomizo, *Physica E* **42**, 2820 (2010)
25. R. Hoffmann, *Angewandte Chemie International Edition* **52**(1), 93 (2013). doi:[10.1002/anie.201206678](https://doi.org/10.1002/anie.201206678). URL <http://dx.doi.org/10.1002/anie.201206678>
26. T. Morishita, K. Nishio, M. Mikami, *Phys. Rev. B* **77**(8), 081401 (2008). doi:[10.1103/PhysRevB.77.081401](https://doi.org/10.1103/PhysRevB.77.081401)
27. G. Liu, M.S. Wu, C.Y. Ouyang, B. Xu, *EPL (Europhys. Lett.)* **99**(1), 17010 (2012). URL: <http://stacks.iop.org/0295-5075/99/i=1/a=17010>
28. T.P. Kaloni, Y.C. Cheng, U. Schwingenschlögl, *J. App. Phys.* **113**, 104305 (2013)
29. B. Wang, J. Wu, X. Gu, H. Yin, Y. Wei, R. Yang, M. Dresselhaus, *Appl. Phys. Lett.* **104**(8), 081902 (2014). Doi:[http://dx.doi.org/10.1063/1.4866415](https://doi.org/10.1063/1.4866415). URL <http://scitation.aip.org/content/aip/journal/apl/104/8/10.1063/1.4866415>
30. C. Yang, Z. Yu, P. Lu, Y. Liu, H. Ye, T. Gao, Phonon instability and ideal strength of silicene under tension. *Comput. Mater. Sci.* **95**(0), 420 (2014). doi:[http://dx.doi.org/10.1016/j.commatsci.2014.07.046](https://doi.org/http://dx.doi.org/10.1016/j.commatsci.2014.07.046). URL <http://www.sciencedirect.com/science/article/pii/S0927025614005291>
31. R. Qin, C.H. Wang, W. Zhu, Y. Zhang, *AIP Adv.* **2**(2), 022159 (2012)

32. V. Bocchetti, H.T. Diep, H. Enriquez, H. Oughaddou, A. Kara, *J. Phys. Conf. Ser.* **491**(1), 012008 (2014). URL <http://stacks.iop.org/1742-6596/491/i=1/a=012008>
33. Y. Zhang, R. Tsu, *Nanoscale Res. Lett.* **5**, 805 (2010)
34. H.S. Sahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akturk, R.T. Senger, S. Ciraci, *Phys. Rev. B* **80**(15), 155453 (2009). doi:[10.1103/PhysRevB.80.155453](https://doi.org/10.1103/PhysRevB.80.155453)
35. H. Zhao, *Phys. Lett. A* **376**(46), 3546 (2012). Doi:[10.1016/j.physleta.2012.10.024](https://doi.org/10.1016/j.physleta.2012.10.024). URL <http://www.sciencedirect.com/science/article/pii/S0375960112010523>
36. R.E. Roman, S.W. Cranford, *Comput. Mater. Sci.* **82**(0), 50 (2014). Doi:<http://dx.doi.org/10.1016/j.commatsci.2013.09.030>. URL <http://www.sciencedirect.com/science/article/pii/S092702561300565X>
37. Z.G. Shao, X.S. Ye, L. Yang, C.L. Wang, *J. Appl. Phys.* **114**(9), 093712 (2013)
38. Q. Lu, M. Arroyo, R. Huang, *J. Phys. D Appl. Phys.* **42**(10), 102002 (2009). URL <http://stacks.iop.org/0022-3727/42/i=10/a=102002>
39. A.C. Ferrari, J.C. Meyer, V. Scardaci, C. Casiraghi, M. Lazzeri, F. Mauri, S. Piscanec, D. Jiang, K.S. Novoselov, S. Roth, A.K. Geim, *Phys. Rev. Lett.* **97**(18), 187401 (2006). doi:[10.1103/PhysRevLett.97.187401](https://doi.org/10.1103/PhysRevLett.97.187401). URL <http://link.aps.org/abstract/PRL/v97/e187401>
40. R. Yan, Q. Zhang, W. Li, I. Calizo, T. Shen, C.A. Richter, A.R. Hight-Walker, X. Liang, A. Seabaugh, D. Jena, H. Grace Xing, D.J. Gundlach, N.V. Nguyen, *Applied Physics Letters* **101**(2), 022105 (2012). doi:<http://dx.doi.org/10.1063/1.4734955>. URL <http://scitation.aip.org/content/aip/journal/apl/101/2/10.1063/1.4734955>
41. H. Xie, M. Hu, H. Bao, *Appl. Phys. Lett.* **104**(13), 131906 (2014). doi:<http://dx.doi.org/10.1063/1.4870586>. URL <http://scitation.aip.org/content/aip/journal/apl/104/13/10.1063/1.4870586>
42. A.A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, C.N. Lau, *Nano Lett.* **8**(3), 902 (2008)
43. Y. Yan, H. Wu, F. Jiang, H. Zhao, *Eur. Phys. J. B* **86**(11), 1 (2013). doi:[10.1140/epjb/e2013-40818-3](https://doi.org/10.1140/epjb/e2013-40818-3). URL <http://dx.doi.org/10.1140/epjb/e2013-40818-3>
44. A.N. Sidorov, A. Sherehiy, R. Jayasinghe, R. Stallard, D.K. Benjamin, Q. Yu, Z. Liu, W. Wu, H. Cao, Y.P. Chen, Z. Jiang, G.U. Sumanasekera, *Appl. Phys. Lett.* **99**(1), 013115 (2011). doi:<http://dx.doi.org/10.1063/1.3609858>. URL <http://scitation.aip.org/content/aip/journal/apl/99/1/10.1063/1.3609858>
45. K. Yang, S. Cahangirov, A. Cantarero, A. Rubio, R. D'Agosta, *Phys. Rev. B* **89**, 125403 (2014). Doi:[10.1103/PhysRevB.89.125403](https://doi.org/10.1103/PhysRevB.89.125403). URL <http://link.aps.org/doi/10.1103/PhysRevB.89.125403>
46. R. Verma, S. Bhattacharya, S. Mahapatra, *IEEE Trans. Electr. Dev.* **60**(6), 2064 (2013). doi:[10.1109/TED.2013.2258159](https://doi.org/10.1109/TED.2013.2258159)
47. Q. Peng, X. Wen, S. De, *RSC Adv.* **3**, 13772 (2013). doi:[10.1039/C3RA41347K](https://doi.org/10.1039/C3RA41347K). URL <http://dx.doi.org/10.1039/C3RA41347K>
48. N.Y. Dzade, K.O. Obodo, S.K. Adjokatse, A.C. Ashu, E. Amankwah, C.D. Atiso, A.A. Bello, E. Igumbor, S.B. Nzabarinda, J.T. Obodo, A.O. Ogbuu, O.E. Femi, J.O. Udeigwe, U. V. Waghmare, *J. Phys. Condens. Matter* **22**, 375502 (2010)
49. R. Qin, W. Zhu, Y. Zhang, X. Deng, *Nano. Res. Lett.* **9**(1), 521 (2014)
50. R. Ansari, S. Rouhi, S. Ajori, *Superlattices Microstruct.* **65**(0), 64 (2014). doi:<http://dx.doi.org/10.1016/j.spmi.2013.10.039>. URL <http://www.sciencedirect.com/science/article/pii/S0749603613003765>
51. Q.X. Pei, Z.D. Sha, Y.Y. Zhang, Y.W. Zhang, *J. Appl. Phys.* **115**(2), 023519 (2014). doi:<http://dx.doi.org/10.1063/1.4861736>. URL <http://scitation.aip.org/content/aip/journal/jap/115/2/10.1063/1.4861736>
52. S. Wang, L. Zhu, Q. Chen, J. Wang, F. Ding, *J. Appl. Phys.* **109**(5), 053516 (2011)
53. M. Houssa, G. Pourtois, V.V. Afanas'ev, A. Stesmans, *Appl. Phys. Lett.* **96**, 082111 (2010)
54. M. Houssa, G. Pourtois, V.V. Afanas'ev, A. Stesmans, *Appl. Phys. Lett.* **97**, 112106 (2010)
55. M. Houssa, G. Pourtois, M.M. Heyns, V.V. Afanas'ev, A. Stesmans, *J. Electrochem. Soc.* **158**(2), H107 (2011)
56. S. Wang, *J. Phys. Soc. Jpn.* **79**, 064602 (2010)

57. R. Arafune, C.L. Lin, R. Nagao, M. Kawai, N. Takagi, *Phys. Rev. Lett.* **110**, 229701 (2013). doi:[10.1103/PhysRevLett.110.229701](https://doi.org/10.1103/PhysRevLett.110.229701). URL <http://link.aps.org/doi/10.1103/PhysRevLett.110.229701>
58. P. Gori, O. Pulci, F. Ronci, S. Colonna, F. Bechsted, *J. Appl. Phys.* **114**(11), 113710 (2013)
59. C.L. Lin, R. Arafune, K. Kawahara, M. Kanno, N. Tsukahara, E. Minamitani, Y. Kim, M. Kawai, N. Takagi, *Phys. Rev. Lett.* **110**, 076801 (2013). doi:[10.1103/PhysRevLett.110.076801](https://doi.org/10.1103/PhysRevLett.110.076801). URL <http://link.aps.org/doi/10.1103/PhysRevLett.110.076801>
60. D. Tsoutsou, E. Xenogiannopoulou, E. Golias, P. Tsipas, A. Dimoulas, *Appl. Phys. Lett.* **103** (23), 231604 (2013). doi:[http://dx.doi.org/10.1063/1.4841335](https://doi.org/10.1063/1.4841335). URL <http://scitation.aip.org/content/aip/journal/apl/103/23/10.1063/1.4841335>
61. M.X. Chen, M. Weinert, *Nano Lett.* doi:[10.1021/nl502107v](https://doi.org/10.1021/nl502107v). URL <http://pubs.acs.org/doi/abs/10.1021/nl502107v>
62. N.W. Johnson, P. Vogt, A. Resta, P. De Padova, I. Perez, D. Muir, E.Z. Kurmaev, G. Le Lay, A. Moewes, *Adv. Funct. Mater.* **24**(33), 5253 (2014). doi:[10.1002/adfm.201400769](https://doi.org/10.1002/adfm.201400769). URL <http://dx.doi.org/10.1002/adfm.201400769>
63. S.K. Mahatha, P. Moras, V. Bellini, P.M. Sheverdyaeva, C. Struzzi, L. Petaccia, C. Carbone, *Phys. Rev. B* **89**, 201416 (2014). DOI [10.1103/PhysRevB.89.201416](https://doi.org/10.1103/PhysRevB.89.201416). URL <http://link.aps.org/doi/10.1103/PhysRevB.89.201416>
64. E. Scalise, E. Cinquanta, M. Houssa, B. van den Broek, D. Chiappe, C. Grazianetti, G. Pourtois, B. Ealet, A. Molle, M. Fanciulli, V. Afanas ev, A. Stesmans, *Appl. Surf. Sci.* **291** (1), 113 (2013). doi:[http://dx.doi.org/10.1016/j.apsusc.2013.08.113](https://doi.org/10.1016/j.apsusc.2013.08.113). URL <http://www.sciencedirect.com/science/article/pii/S0169433213016048>
65. H. Ishida, Y. Hamamoto, Y. Morikawa, E. Minamitani, R. Arafune, N. Takagi, *New J. Phys.* **17**(1), 015013 (2015). URL <http://stacks.iop.org/1367-2630/17/i=1/a=015013>
66. L. Chen, C.C. Liu, B. Feng, X. He, P. Cheng, Z. Ding, S. Meng, Y. Yao, K. Wu, *Phys. Rev. Lett.* **109**, 056804 (2012). doi:[10.1103/PhysRevLett.109.056804](https://doi.org/10.1103/PhysRevLett.109.056804). URL <http://link.aps.org/doi/10.1103/PhysRevLett.109.056804>
67. B. Feng, H. Li, C.C. Liu, T.N. Shao, P. Cheng, Y. Yao, S. Meng, L. Chen, K. Wu, *ACS Nano* **7**(10), 9049 (2013). doi:[10.1021/nn403661h](https://doi.org/10.1021/nn403661h). URL <http://pubs.acs.org/doi/abs/10.1021/nn403661h>
68. C.C. Liu, W. Feng, Y. Yao, *Phys. Rev. Lett.* **107**, 076802 (2011). doi:[10.1103/PhysRevLett.107.076802](https://doi.org/10.1103/PhysRevLett.107.076802). URL <http://link.aps.org/doi/10.1103/PhysRevLett.107.076802>
69. F. Geissler, J.C. Budich, B. Trauzettel, *New J. Phys.* **15**(8), 085030 (2013). URL <http://stacks.iop.org/1367-2630/15/i=8/a=085030>
70. L.C.L.Y. Voon, A. Lopez-Bezanilla, J. Wang, Y. Zhang, M. Willatzen, *New J. Phys.* **17**(2), 025004 (2015). URL <http://stacks.iop.org/1367-2630/17/i=2/a=025004>
71. R. Winkler, U. Zülicke, *Phys. Rev. B* **82**, 245313 (2010). doi:[10.1103/PhysRevB.82.245313](https://doi.org/10.1103/PhysRevB.82.245313). URL <http://link.aps.org/doi/10.1103/PhysRevB.82.245313>
72. M. Ezawa, *Phys. Rev. B* **87**, 155415 (2013). doi:[10.1103/PhysRevB.87.155415](https://doi.org/10.1103/PhysRevB.87.155415). URL <http://link.aps.org/doi/10.1103/PhysRevB.87.155415>
73. Y. Wang, Y. Ding, *Solid State Commun.* **155**(2), 6 (2013)
74. A. Durajski, D. Szczes'niak, R. Szczes'niak, *Solid State Commun.* **200**, 17 (2014). doi:[http://dx.doi.org/10.1016/j.ssc.2014.09.007](https://doi.org/10.1016/j.ssc.2014.09.007). URL <http://www.sciencedirect.com/science/article/pii/S0038109814003664>
75. B. Mohan, A. Kumar, P. Ahluwalia, *Physica E: Low-dimensional systems and nanostructures* **61**(0), 40 (2014). doi:[http://dx.doi.org/10.1016/j.physe.2014.03.013](https://doi.org/10.1016/j.physe.2014.03.013). URL <http://www.sciencedirect.com/science/article/pii/S1386947714001003>
76. C.H. Yang, Z.Y. Yu, P.F. Lu, Y.m. Liu, S. Manzoor, M. Li, S. Zhou, *Proc. SPIE* **8975**, 89750K (2014). doi:[10.1117/12.2038401](https://doi.org/10.1117/12.2038401). URL <http://dx.doi.org/10.1117/12.2038401>
77. Z. Ni, Q. Liu, K. Tang, J. Zheng, J. Zhou, R. Qin, Z. Gao, D. Yu, J. Lu, *Nano Lett.* **12**(1), 113 (2012). doi:[10.1021/nl203065e](https://doi.org/10.1021/nl203065e). URL <http://pubs.acs.org/doi/abs/10.1021/nl203065e>
78. N.D. Drummond, V. Zólyomi, V.I. Fal'ko, *Phys. Rev. B* **85**, 075423 (2012). doi:[10.1103/PhysRevB.85.075423](https://doi.org/10.1103/PhysRevB.85.075423). URL <http://link.aps.org/doi/10.1103/PhysRevB.85.075423>

79. V. Vargiamidis, P. Vasilopoulos, G.Q. Hai, J. Phys. Condens. Matter **26**(34), 345303 (2014). URL <http://stacks.iop.org/0953-8984/26/i=34/a=345303>
80. C.L. Kane, E.J. Mele, Phys. Rev. Lett. **95**, 226801 (2005). doi:10.1103/PhysRevLett.95.226801. URL <http://link.aps.org/doi/10.1103/PhysRevLett.95.226801>
81. M. Ezawa, Eur. J. Phys. B **85**(11), 1 (2012)
82. C.L. Kane, E.J. Mele, Phys. Rev. Lett. **95**, 146802 (2005). doi:10.1103/PhysRevLett.95.146802. URL <http://link.aps.org/doi/10.1103/PhysRevLett.95.146802>
83. M. Tahir, U. Schwingenschlogl, Sci. Rep. **3**(1075), 1 (2013)
84. M. Tahir, A. Manchon, K. Sabeeh, U. Schwingenschlogl, Appl. Phys. Lett. **102**(16), 162412 (2013)
85. M. Ezawa, New J. Phys. **14**(3), 033003 (2012). URL <http://stacks.iop.org/1367-2630/14/i=3/a=033003>
86. M. Ezawa, Phys. Rev. Lett. **110**, 026603 (2013). doi:10.1103/PhysRevLett.110.026603. URL <http://link.aps.org/doi/10.1103/PhysRevLett.110.026603>
87. M. Ezawa, JPS Conf. Proc. **1**(1), 012003 (2014)
88. Y. Kim, K. Choi, J. Ihm, H. Jin, Phys. Rev. B **89**, 085429 (2014). doi:10.1103/PhysRevB.89.085429. URL <http://link.aps.org/doi/10.1103/PhysRevB.89.085429>
89. S.K. Wang, J. Wang, K.S. Chan, New J. Phys. **16**(4), 045015 (2014). URL <http://stacks.iop.org/1367-2630/16/i=4/a=045015>
90. D.Q. Fang, S.L. Zhang, H. Xu, RSC Adv. **3**, 24075 (2013). doi:10.1039/C3RA42720J. URL <http://dx.doi.org/10.1039/C3RA42720J>
91. H.X. Luan, C.W. Zhang, F.B. Zheng, P.J. Wang, J. Phys. Chem. C. doi:10.1021/jp4005357. URL <http://pubs.acs.org/doi/abs/10.1021/jp4005357>
92. L. Ma, J.M. Zhang, K.W. Xu, V. Ji, Phys. B **425**, 66 (2013)
93. F. Zheng, C. Zhang, P. Wang, S. Li, J. Appl. Phys. **113**(15), 154302 (2013)
94. F. Zheng, C. Zhang, S. Yan, F. Li, J. Mater. Chem. C **1**, 2735 (2013). doi:10.1039/C3TC30097H. URL <http://dx.doi.org/10.1039/C3TC30097H>
95. A.B. Chen, X.F. Wang, P. Vasilopoulos, M.X. Zhai, Y.S. Liu, Phys. Chem. Chem. Phys. **16**, 5113 (2014). doi:10.1039/C3CP55447C. URL <http://dx.doi.org/10.1039/C3CP55447C>
96. J. Chen, X.F. Wang, P. Vasilopoulos, A.B. Chen, J.C. Wu, ChemPhysChem **15**(13), 2701 (2014). doi:10.1002/cphc.201402171. URL <http://dx.doi.org/10.1002/cphc.201402171>
97. Y.J. Dong, X.F. Wang, P. Vasilopoulos, M.X. Zhai, X.M. Wu, J. Phys. D Appl. Phys. **47**(10), 105304 (2014). URL <http://stacks.iop.org/0022-3727/47/i=10/a=105304>
98. Y. Liu, X. Yang, X. Zhang, X. Hong, X.F. Wang, J. Feng, C. Zhang, RSC Adv. (2014). doi:10.1039/C4RA07791A. URL <http://dx.doi.org/10.1039/C4RA07791A>
99. A. Lopez-Bezanilla, J. Phys. Chem. C **118**(32), 18788 (2014). doi:10.1021/jp5060809. URL <http://dx.doi.org/10.1021/jp5060809>
100. L. Ma, J.M. Zhang, K.W. Xu, V. Ji, Phys. E Low-Dimension. Syst. Nanostruct. **60**(0), 112 (2014). doi:http://dx.doi.org/10.1016/j.physe.2014.02.013. URL <http://www.sciencedirect.com/science/article/pii/S1386947714000642>
101. J.M. Zhang, W.T. Song, K.W. Xu, V. Ji, Comput. Mater. Sci. **95**(0), 429 (2014). doi:http://dx.doi.org/10.1016/j.commatsci.2014.08.019. URL <http://www.sciencedirect.com/science/article/pii/S0927025614005618>
102. X. Pi, Z. Ni, Y. Liu, Z. Ruan, M. Xu, D. Yang, Phys. Chem. Chem. Phys. **17**, 4146 (2015). doi:10.1039/C4CP05196C. URL <http://dx.doi.org/10.1039/C4CP05196C>
103. X. Tan, F. Li, Z. Chen, J. Phys. Chem. C **118**(45), 25825 (2014). doi:10.1021/jp507011p. URL <http://dx.doi.org/10.1021/jp507011p>
104. A. Manjanath, V. Kumar, A.K. Singh, Phys. Chem. Chem. Phys. **16**, 1667 (2014). doi:10.1039/C3CP54655A. URL <http://dx.doi.org/10.1039/C3CP54655A>
105. Y.C. Cheng, Z.Y. Zhu, U. Schwingenschlöggl, Europhys. Lett. **95**, 17005 (2011)
106. R.R. Nair, P. Blake, A.N. Grigorenko, K.S. Novoselov, T.J. Booth, T. Stauber, N.M.R. Peres, A.K. Geim, Science **320**(5881), 1308 (2008)
107. F. Bechstedt, L. Matthes, P. Gori, O. Pulci, Appl. Phys. Lett. **100**, 261906 (2012)

108. L. Matthes, P. Gori, O. Pulci, F. Bechstedt, *Phys. Rev. B* **87**, 035438 (2013). doi:[10.1103/PhysRevB.87.035438](https://doi.org/10.1103/PhysRevB.87.035438). URL <http://link.aps.org/doi/10.1103/PhysRevB.87.035438>
109. L. Matthes, O. Pulci, F. Bechstedt, *J. Phys. Cond. Matter* **25**, 395305 (2013)
110. L. Matthes, O. Pulci, F. Bechstedt, *New J. Phys.* **16**(10), 105007 (2014). URL <http://stacks.iop.org/1367-2630/16/i=10/a=105007>
111. H. Bao, J. Guo, W. Liao, H. Zhao, *Appl. Phys. A*, 1–5 (2014). doi:[10.1007/s00339-014-8837-x](https://doi.org/10.1007/s00339-014-8837-x). URL <http://dx.doi.org/10.1007/s00339-014-8837-x>
112. B. Mohan, A. Kumar, P. Ahluwalia, *Phys. E: Low-Dimension. Syst. Nanostruct.* **53**, 233 (2013). doi:[10.1016/j.physe.2013.05.014](https://doi.org/10.1016/j.physe.2013.05.014). URL <http://www.sciencedirect.com/science/article/pii/S1386947713001872>
113. C.J. Tabert, E.J. Nicol, *Phys. Rev. B* **89**, 195410 (2014). doi:[10.1103/PhysRevB.89.195410](https://doi.org/10.1103/PhysRevB.89.195410). URL <http://link.aps.org/doi/10.1103/PhysRevB.89.195410>
114. H.R. Chang, J. Zhou, H. Zhang, Y. Yao, *Phys. Rev. B* **89**, 201411 (2014). doi:[10.1103/PhysRevB.89.201411](https://doi.org/10.1103/PhysRevB.89.201411). URL <http://link.aps.org/doi/10.1103/PhysRevB.89.201411>
115. J.Y. Wu, S.C. Chen, M.F. Lin, *New J. Phys.* **16**(12), 125002 (2014). URL <http://stacks.iop.org/1367-2630/16/i=12/a=125002>
116. R. Das, S. Chowdhury, A. Majumdar, D. Jana, *RSC Adv.* **5**, 41 (2015). doi:[10.1039/C4RA07976K](https://doi.org/10.1039/C4RA07976K). URL <http://dx.doi.org/10.1039/C4RA07976K>
117. Y. Yao, S.Y. Liu, X.L. Lei, *Phys. Rev. B* **91**, 115411 (2015). doi:[10.1103/PhysRevB.91.115411](https://doi.org/10.1103/PhysRevB.91.115411). URL <http://link.aps.org/doi/10.1103/PhysRevB.91.115411>
118. C.J. Tabert, E.J. Nicol, *Phys. Rev. Lett.* **110**, 197402 (2013). doi:[10.1103/PhysRevLett.110.197402](https://doi.org/10.1103/PhysRevLett.110.197402). URL <http://link.aps.org/doi/10.1103/PhysRevLett.110.197402>
119. C.J. Tabert, E.J. Nicol, *Phys. Rev. B* **88**, 085434 (2013). doi:[10.1103/PhysRevB.88.085434](https://doi.org/10.1103/PhysRevB.88.085434). URL <http://link.aps.org/doi/10.1103/PhysRevB.88.085434>
120. N. Singh, U. Schwingenschlgl, *Phys. Status Solidi (RRL) Rapid Res. Lett.* **8**(4) (2014). doi:[10.1002/pssr.201409025](https://doi.org/10.1002/pssr.201409025). URL <http://dx.doi.org/10.1002/pssr.201409025>
121. V.Y. Tsaran, S.G. Sharapov, *Phys. Rev. B* **90**, 205417 (2014). doi:[10.1103/PhysRevB.90.205417](https://doi.org/10.1103/PhysRevB.90.205417). URL <http://link.aps.org/doi/10.1103/PhysRevB.90.205417>
122. C.P. Chang, *J. Appl. Phys.* **110**(1), 013725 (2011). doi:[http://dx.doi.org/10.1063/1.3603040](https://doi.org/10.1063/1.3603040). URL <http://scitation.aip.org/content/aip/journal/jap/110/1/10.1063/1.3603040>
123. J.M. Luttinger, W. Kohn, *Phys. Rev.* **97**(4), 869 (1955)
124. V.P. Gusynin, S.G. Sharapov, J.P. Carbotte, *Phys. Rev. Lett.* **98**, 157402 (2007). doi:[10.1103/PhysRevLett.98.157402](https://doi.org/10.1103/PhysRevLett.98.157402). URL <http://link.aps.org/doi/10.1103/PhysRevLett.98.157402>
125. Y. Zhang, Y.W. Tan, H.L. Stormer, P. Kim, *Nature* **438**, 201 (2005)
126. Y. Zhang, Z. Jiang, J.P. Small, M.S. Purewal, Y.W. Tan, M. Fazlollahi, J.D. Chudow, J.A. Jaszczak, H.L. Stormer, P. Kim, *Phys. Rev. Lett.* **96**, 136806 (2006). doi:[10.1103/PhysRevLett.96.136806](https://doi.org/10.1103/PhysRevLett.96.136806). URL <http://link.aps.org/doi/10.1103/PhysRevLett.96.136806>
127. Z. Jiang, E.A. Henriksen, L.C. Tung, Y.J. Wang, M.E. Schwartz, M.Y. Han, P. Kim, H.L. Stormer, *Phys. Rev. Lett.* **98**, 197403 (2007). doi:[10.1103/PhysRevLett.98.197403](https://doi.org/10.1103/PhysRevLett.98.197403). URL <http://link.aps.org/doi/10.1103/PhysRevLett.98.197403>
128. K. Shakouri, P. Vasilopoulos, V. Vargiamidis, F.M. Peeters, *Phys. Rev. B* **90**, 235423 (2014). doi:[10.1103/PhysRevB.90.235423](https://doi.org/10.1103/PhysRevB.90.235423). URL <http://link.aps.org/doi/10.1103/PhysRevB.90.235423>
129. N.J. Roome, J.D. Carey, *ACS Appl. Mater. Interfaces*. doi:[10.1021/am501022x](https://doi.org/10.1021/am501022x). URL <http://pubs.acs.org/doi/abs/10.1021/am501022x>
130. G. Berdiyrov, F. Peeters, *RSC Adv.* **4**(3), 1133 (2014)
131. H. peng Li, R. qin Zhang, *EPL (Europhy. Lett.)* **99**(3), 36001 (2012). URL <http://stacks.iop.org/0295-5075/99/i=3/a=36001>
132. L. Wang, H. Sun, *J. Mol. Model.* **18**, 4811 (2012). URL <http://dx.doi.org/10.1007/s00894-012-1482-4>. [10.1007/s00894-012-1482-4](https://doi.org/10.1007/s00894-012-1482-4)
133. M. Hu, X. Zhang, D. Poulidakos, *Phys. Rev. B* **87**, 195417 (2013). doi:[10.1103/PhysRevB.87.195417](https://doi.org/10.1103/PhysRevB.87.195417). URL <http://link.aps.org/doi/10.1103/PhysRevB.87.195417>
134. Q.X. Pei, Y.W. Zhang, Z.D. Sha, V.B. Shenoy, *J. Appl. Phys.* **114**(3), 033526 (2013). doi:[10.1063/1.4815960](https://doi.org/10.1063/1.4815960)

135. T. Ng, J. Yeo, Z. Liu, *Int.J. Mech. Mater. Des.* **9**, 105 (2013). doi:[10.1007/s10999-013-9215-0](https://doi.org/10.1007/s10999-013-9215-0). URL <http://dx.doi.org/10.1007/s10999-013-9215-0>
136. B. Liu, C.D. Reddy, J. Jiang, H. Zhu, J.A. Baimova, S.V. Dmitriev, K. Zhou, *J. Phys. D Appl. Phys.* **47**(16), 165301 (2014). URL <http://stacks.iop.org/0022-3727/47/i=16/a=165301>
137. J.J. Yeo, Z.S. Liu, *J. Comput. Theor. Nanosci.* **11**(8), 1790 (2014-08-01T00:00:00). doi:[10.1166/jctn.2014.3568](https://doi.org/10.1166/jctn.2014.3568). URL <http://www.ingentaconnect.com/content/asp/jctn/2014/00000011/00000008/art00011>
138. X. Zhang, H. Xie, M. Hu, H. Bao, S. Yue, G. Qin, G. Su, *Phys. Rev. B* **89**, 054310 (2014). doi:[10.1103/PhysRevB.89.054310](https://doi.org/10.1103/PhysRevB.89.054310). URL <http://link.aps.org/doi/10.1103/PhysRevB.89.054310>
139. Z. Wang, T. Feng, X. Ruan, *J. Appl. Phys.* **117**(8), 084317 (2015). doi:[http://dx.doi.org/10.1063/1.4913600](https://doi.org/http://dx.doi.org/10.1063/1.4913600). URL <http://scitation.aip.org/content/aip/journal/jap/117/8/10.1063/1.4913600>
140. X. Zhang, H. Bao, M. Hu, *Nanoscale* **7**, 6014 (2015). Doi:[10.1039/C4NR06523A](https://doi.org/10.1039/C4NR06523A). URL <http://dx.doi.org/10.1039/C4NR06523A>
141. M. Kamatagi, J. Elliott, N. Sankeshwar, A. Lindsay Greer, in *Physics of Semiconductor Devices*, ed. by V.K. Jain, A. Verma, Environmental science and engineering (Springer International Publishing, 2014), pp. 617–619. doi:[10.1007/978-3-319-03002-9_157](https://doi.org/10.1007/978-3-319-03002-9_157). URL http://dx.doi.org/10.1007/978-3-319-03002-9_157
142. B. Liu, J.A. Baimova, C.D. Reddy, S.V. Dmitriev, W.K. Law, X.Q. Feng, K. Zhou, *Carbon* **79**(0), 236 (2014). doi:[http://dx.doi.org/10.1016/j.carbon.2014.07.064](https://doi.org/http://dx.doi.org/10.1016/j.carbon.2014.07.064). URL <http://www.sciencedirect.com/science/article/pii/S0008622314007027>
143. G. Liu, X.L. Lei, M.S. Wu, B. Xu, C.Y. Ouyang, *EPL (Europhys. Lett.)* **106**(4), 47001 (2014). URL <http://stacks.iop.org/0295-5075/106/i=4/a=47001>
144. G. Liu, X.L. Lei, M.S. Wu, B. Xu, C.Y. Ouyang, *J. Phys. Condens. Matter* **26**(35), 355007 (2014). URL <http://stacks.iop.org/0953-8984/26/i=35/a=355007>
145. Y. Du, J. Zhuang, H. Liu, X. Xu, S. Eilers, K. Wu, P. Cheng, J. Zhao, X. Pi, K.W. See, G. Peleckis, X. Wang, S.X. Dou, *ACS Nano* **8**(10), 10019 (2014). doi:[10.1021/nn504451t](https://doi.org/10.1021/nn504451t). URL <http://dx.doi.org/10.1021/nn504451t>. PMID: 25248135
146. V.O. Özçelik, H.H. Gurel, S. Ciraci, *Phys. Rev. B* **88**, 045440 (2013). doi:[10.1103/PhysRevB.88.045440](https://doi.org/10.1103/PhysRevB.88.045440). URL <http://link.aps.org/doi/10.1103/PhysRevB.88.045440>
147. R. Li, Y. Han, T. Hu, J. Dong, Y. Kawazoe, *Phys. Rev. B* **90**, 045425 (2014). doi:[10.1103/PhysRevB.90.045425](https://doi.org/10.1103/PhysRevB.90.045425). URL <http://link.aps.org/doi/10.1103/PhysRevB.90.045425>
148. J. Gao, J. Zhang, H. Liu, Q. Zhang, J. Zhao, *Nanoscale* **5**, 9785 (2013). doi:[10.1039/C3NR02826G](https://doi.org/10.1039/C3NR02826G). URL <http://dx.doi.org/10.1039/C3NR02826G>
149. S. Li, Y. Wu, Y. Tu, Y. Wang, T. Jiang, W. Liu, Y. Zhao, *Sci. Rep.* **5**(7881) (2015)
150. A. Manjanath, A.K. Singh, *Chem. Phys. Lett.* **592**(0), 52 (2014). doi:[10.1016/j.cplett.2013.12.010](https://doi.org/10.1016/j.cplett.2013.12.010). URL <http://www.sciencedirect.com/science/article/pii/S0009261413014905>
151. V.V. Hoang, H.T.C. Mi, *J. Phys. D Appl. Phys.* **47**(49), 495303 (2014). URL <http://stacks.iop.org/0022-3727/47/i=49/a=495303>
152. M.Q. Le, D.T. Nguyen, *Appl. Phys. A*, 1–9 (2014). doi:[10.1007/s00339-014-8904-3](https://doi.org/10.1007/s00339-014-8904-3). URL <http://dx.doi.org/10.1007/s00339-014-8904-3>
153. M.P. Lima, A. Fazzio, A.J.R. da Silva, *Phys. Rev. B* **88**, 235413 (2013). doi:[10.1103/PhysRevB.88.235413](https://doi.org/10.1103/PhysRevB.88.235413). URL <http://link.aps.org/doi/10.1103/PhysRevB.88.235413>
154. M. Ezawa, *Phys. Rev. Lett.* **109**, 055502 (2012)
155. P. Gori et al., Thermophysical properties of the novel 2D materials graphene and silicene: insights from Ab initio calculations. *Energy Proc.* **45**, 512 (2014)

Silicene

Structure, Properties and Applications

Spencer, M.; Morishita, T. (Eds.)

2016, XVI, 276 p. 149 illus., 102 illus. in color.,

Hardcover

ISBN: 978-3-319-28342-5