

RESEARCH ARTICLE

Structural Stability, Electronic Band Structure, and Spin–Orbit Coupling Effects in Two–Dimensional Stanene

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ABSTRACT: This study investigates the structural and electronic properties of monolayer stanene, a two-dimensional honeycomb material composed of tin atoms. The calculations were performed within the framework of density functional theory as implemented in the Quantum ESPRESSO package. We systematically examined the total energy convergence, lattice constant relaxation, and k-point sampling to ensure reliable predictions. The optimized geometry reveals a low-buckled honeycomb structure rather than a perfectly planar one, which is found to be energetically more stable. The calculated lattice constant, bond length, and buckling height are in good agreement with previously reported theoretical and experimental values. The electronic band structure without spin-orbit coupling shows linear dispersion near the high symmetry K and K' points, similar to graphene, indicating that charge carriers behave as massless Dirac fermions. In this case, stanene exhibits a gapless semimetallic character. However, when spin-orbit coupling is included, a direct band gap opens at the Dirac point, transforming stanene into a topological insulator with potential for dissipationless electronic transport. The total and partial density of states further confirm the semimetallic nature and highlight the dominant contribution of pz orbitals near the Fermi level. The mixed sp²–sp³ hybridization due to buckling is responsible for the deviation from ideal planar symmetry. Our computed results align well with existing literature, validating the accuracy of our computational approach. Overall, this work provides a clear understanding of how structural buckling and spin-orbit coupling together govern the electronic behavior of stanene, making it a promising candidate for future nanoelectronic and spintronic devices.

Keywords: Stanene, Density functional theory, Spin orbit coupling, E band structure, Two dimensional materials, Buckling

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1. INTRODUCTION

Over the past decade and a half, the discovery of graphene has fundamentally changed how researchers think about materials at the nanoscale. What started as an experimental curiosity involving Scotch tape and a piece of graphite has grown into a vast field dedicated to two dimensional crystals

[1]. The reason for such widespread interest is not hard to see. Graphene exhibits a remarkable electronic structure where electrons near the Fermi level behave not as ordinary massive particles but as massless Dirac fermions, leading to extremely high mobility and a host of unusual transport phenomena [2–4]. However, graphene has a major limitation for certain applications. It lacks an electronic band gap, which makes it difficult to switch off currents in transistor devices. This single drawback has driven the search for other two dimensional materials that can combine the favorable properties of graphene with a usable band gap.

Among the most promising candidates are the group IV elemental analogues of graphene, namely silicene, germanene, and stanene [5]. These materials share the same

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honeycomb lattice as graphene but are composed of heavier atoms from the same column of the periodic table. As one moves from carbon to silicon to germanium and finally to tin, the atomic size increases and the degree of buckling in the two dimensional sheet also increases. Graphene is perfectly planar, but silicene shows a small buckling, germanene shows a larger one, and stanene exhibits the most pronounced buckled structure. This buckling is not merely a geometric curiosity. It fundamentally alters the electronic properties by mixing sp^2 and sp^3 hybridization, which in turn influences how the pz orbitals interact and how strongly the material couples to external electric fields or substrates.

Stanene, the tin based analogue, has emerged as particularly exciting within this family. Theoretical predictions have suggested that stanene may behave as a topological insulator with a band gap large enough to be useful at room temperature [6, 7]. Topological insulators are a class of materials that conduct electricity on their surfaces or edges while remaining insulating in their interior. This property arises from strong spin orbit coupling, which in stanene is much larger than in graphene, silicene, or germanene simply because tin is a heavy element. The promise of dissipationless electronic transport has sparked considerable research into stanene and its derivatives. Beyond topological insulating behavior, stanene has also been predicted to exhibit the near room temperature quantum anomalous Hall effect [8], topological superconductivity when brought into contact with a superconductor [9], and enhanced thermoelectric performance compared to other two dimensional materials [7]. Each of these predictions points toward stanene being more than just a heavier copy of graphene.

The novelty of the present work lies in a careful, systematic re-examination of stanene's structural and electronic properties using density functional theory without relying on overly simplified tight binding models or assumptions about the strength of spin orbit coupling. While previous studies have reported band structures and lattice parameters, there remains a need for a clear, step by step demonstration of how convergence parameters, lattice relaxation, and the choice of pseudopotentials affect the final results. Many earlier calculations have either ignored spin orbit coupling entirely or treated it as a small perturbation, but for stanene, spin orbit coupling is far from negligible. In this paper, we show explicitly how the inclusion of spin orbit coupling opens a direct band gap at the Dirac point, transforming stanene from a gapless semimetal into a gapped topological insulator. Furthermore, we provide a detailed analysis of the density of states and the partial density of states to identify which atomic orbitals contribute most significantly near the Fermi level. This level of detail helps clarify the role of pz versus pxy orbitals and the degree of sp^2 - sp^3 mixing in the buckled structure. Our results confirm and extend earlier findings, offering a self-contained reference for researchers interested in using stanene for nanoelectronic or spintronic applications.

Understanding the crystal structure is the first step toward controlling any material's properties. Symmetry,

bonding characteristics, and orbital hybridization all originate from the atomic arrangement [5]. In two dimensional group IV materials, the pz orbital is primarily responsible for the electronic behavior near the Fermi level, while the in plane sigma bonds provide mechanical strength. The presence of buckling in stanene offers a practical advantage as well. It allows the material to be integrated with various substrates without destroying its electronic properties, which is a serious challenge for planar graphene. Therefore, determining the precise structural parameters, including the lattice constant, bond length, and buckling height, is essential before any reliable electronic structure calculation can be performed. These parameters will be discussed in detail in the following sections.

The electronic band structure of any solid describes the relationship between electron energy and the crystal momentum vector in reciprocal space. This relationship determines whether a material behaves as a metal, a semiconductor, or an insulator [6]. The position of the Fermi level is particularly important. If the Fermi level lies inside a forbidden energy gap, the material is either insulating or semiconducting depending on the size of the gap. If it lies within a band, the material is metallic. A tunable band gap is highly desirable for device applications because it allows engineers to control whether a transistor is on or off. Stanene's band structure, like that of graphene, shows linear dispersion near the high symmetry K and K' points, meaning that charge carriers near these points behave as massless Dirac fermions. However, unlike graphene, stanene's buckled structure and strong spin orbit coupling introduce a gap at exactly these Dirac points. In this introduction, we set the stage for a detailed investigation of the structural parameters, geometrical stability, electronic band structure, total density of states, and partial density of states of two dimensional monolayer stanene, first without spin orbit coupling to establish a baseline and then with spin orbit coupling to reveal the gap opening. The computational methods are described next, followed by the results and a discussion of their implications.

2. COMPUTATIONAL METHOD

All calculations in this work were performed using density functional theory as implemented in the Quantum ESPRESSO package [10, 11]. Stanene, being a two dimensional material, has a primitive unit cell that contains two tin atoms arranged in a buckled honeycomb lattice. The first step in any reliable DFT study is to ensure that the numerical parameters are chosen carefully enough to give converged results. We therefore carried out systematic convergence tests for the plane wave kinetic energy cutoff, the k point sampling grid, and the in plane lattice constant. These convergence curves are shown in Figure 1 (a), (b), and (c) respectively.

Figure 1 (a) displays the total energy as a function of the plane wave kinetic energy cutoff. As the cutoff increases, the total energy decreases and eventually saturates. Based on this

test, we selected a cutoff of 50 Ry, which provides a good balance between computational cost and numerical accuracy. Figure 1 (b) shows the total energy variation with respect to the in plane lattice constant. The energy minimum occurs at a lattice constant of approximately 4.67 Å, which we adopted for all subsequent calculations. Figure 1 (c) illustrates the convergence of total energy with respect to the k point mesh. A Monkhorst Pack grid of $11 \times 11 \times 1$ was found to be sufficient, as further increasing the grid density changed the total energy by less than 1 meV per unit cell.

Geometry optimization was performed using the Broyden Fletcher Goldfarb Shanno method, which iteratively updates atomic positions until the forces on each atom become negligibly small. The convergence threshold for atomic forces was set to 0.000336 Ry/bohr. The total energy was converged to within 10^{-6} Ry between self-consistent field iterations. For the exchange correlation functional, we used the Perdew Burke Ernzerhof parametrization within the generalized gradient approximation. An ultrasoft pseudopotential with scalar relativistic correction was employed to describe the core electrons of tin. Since stanene is a two dimensional sheet, we introduced a vacuum spacing of 30 Å along the direction perpendicular to the plane to eliminate any spurious interactions between periodic images. It is important to note that the calculations described in this section were performed without including spin orbit coupling. The reason for this is to first establish a baseline understanding of the structural and electronic properties before examining the additional effects introduced by spin orbit coupling, which will be discussed separately in the following sections.

3. RESULTS AND DISCUSSION

3.1. Structure Parameters

The optimized structural parameters of monolayer stanene were obtained using the computational methods described in the previous section. After full geometry relaxation, the stable configuration of stanene was determined and is illustrated in Figures 2(a)-(e). These figures present different perspectives of the two dimensional tin honeycomb lattice, allowing a clear visualization of its characteristic buckled geometry.

Figure 2(a) shows a perspective view of the stanene monolayer from an oblique angle. This view clearly reveals the buckled nature of the structure, where the two triangular sublattices are displaced vertically relative to each other. Figure 2(b) presents a side view along one of the in plane directions, making the buckling height directly visible as the vertical separation between the two sublattices. Figure 2(c) displays a top view looking straight down onto the plane, which shows the perfect hexagonal honeycomb arrangement similar to graphene when projected onto two dimensions. Figures 2(d) and 2(e) provide additional rotated and magnified views to highlight the bonding geometry and the relative positions of neighboring tin atoms.

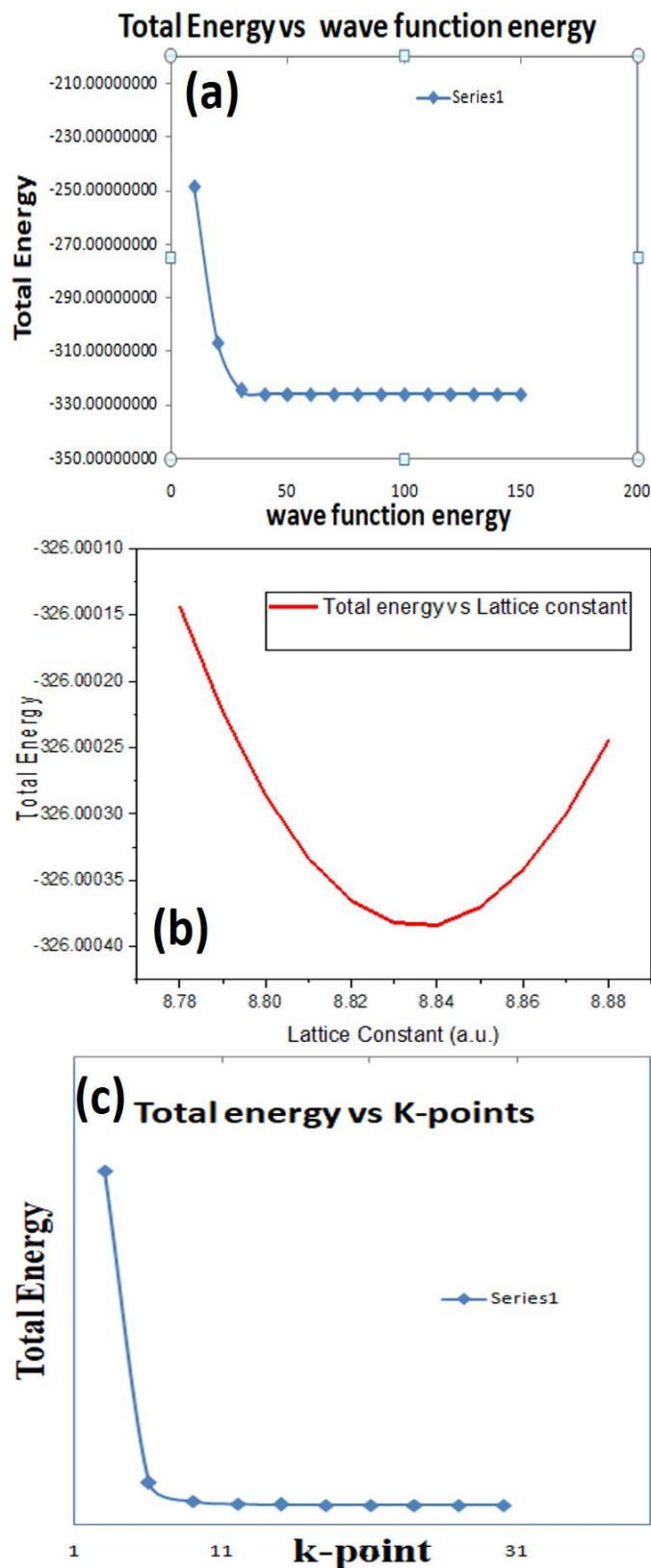


Fig. 1. Convergence tests for monolayer stanene: (a) total energy versus plane wave kinetic energy cutoff in Ry, showing saturation beyond 50 Ry; (b) total energy versus in plane lattice constant in Ångströms, with the minimum energy occurring at 4.67 Å; (c) total energy versus k point grid density, demonstrating convergence with an $11 \times 11 \times 1$ Monkhorst Pack mesh.

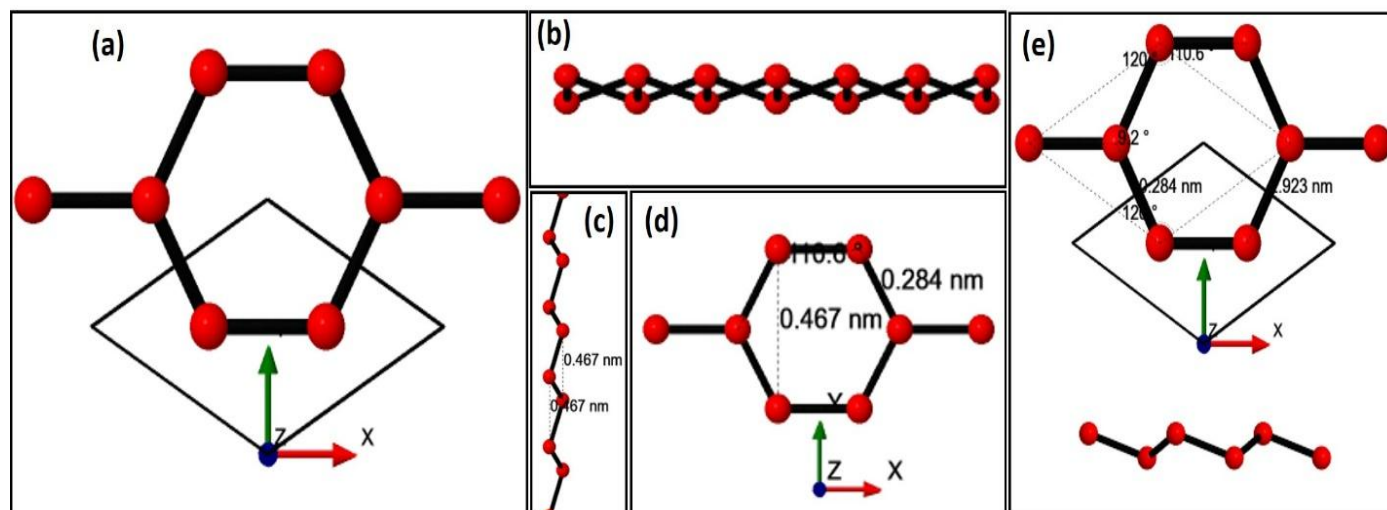


Fig. 2. Optimized geometry of monolayer stanene shown from multiple perspectives: (a) oblique perspective view illustrating the overall buckled honeycomb lattice; (b) side view clearly displaying the vertical buckling height between the two triangular sublattices; (c) top view along the perpendicular direction showing the hexagonal ring arrangement; (d) rotated perspective highlighting the bonding angles and nearest neighbor distances; (e) magnified side view emphasizing the relative displacement of adjacent tin atoms.

From these optimized structures, we extracted the key geometric parameters. The calculated lattice constant is 4.67 Å, the nearest neighbor bond length is 2.82 Å, and the buckling height, which is the vertical distance between the two sublattices, is 0.85 Å. These values are in excellent agreement with previously reported theoretical and experimental results [12–16]. It is worth noting that the bond length we obtained is larger than that of graphene, which is expected because tin atoms are considerably larger than carbon atoms.

Unlike graphene, where the two triangular sublattices lie perfectly in the same plane, stanene exhibits a low buckled configuration. One sublattice is slightly raised relative to the other, and this vertical separation is precisely the buckling height of 0.85 Å [14, 17]. This asymmetry serves an important purpose. It removes the mechanical instability that plagues planar honeycomb structures composed of heavier elements. In other words, if we tried to force stanene into a perfectly flat geometry, it would be energetically unfavorable and would likely distort spontaneously. The presence of this low buckling also has profound consequences for the electronic properties, as will be discussed later.

The bond angle in stanene was computed to be 110.6 degrees using auxiliary quantum chemical software. This value is notably smaller than the 120 degree bond angle found in graphene. The significance of this difference lies in what it tells us about orbital hybridization. Graphene exhibits pure sp^2 hybridization, which naturally gives 120 degree bond angles and a planar geometry. Stanene, with its bond angle of 110.6 degrees, is much closer to the ideal tetrahedral angle of 109.5 degrees that characterizes sp^3 hybridization. This indicates that stanene prefers a mixed sp^2 – sp^3 hybridization rather than pure sp^2 [18]. As a result, stanene

adopts a low buckled honeycomb structure instead of a planar one.

Another important consequence of buckling concerns the nature of π bonding. In a perfectly planar structure, the p_z orbitals of adjacent atoms align parallel to each other, allowing strong π bonding between nearest neighbors. However, in the buckled structure of stanene, the lobes of adjacent atoms point in slightly different directions. This geometric arrangement favors π bonding with next nearest neighbors rather than with nearest neighbors. The orbitals tend to hybridize into sp^3 like configurations rather than remaining as sp^2 , which weakens the π bonds and stabilizes the buckled geometry. In simple terms, the presence of buckling stabilizes the sigma bonds while destabilizing the pi bonds. Regarding symmetry, monolayer stanene belongs to the space group D_{3d}^3 ($\bar{p}3m1$) and the point group D_{3d} ($\bar{3}m$), both of which include inversion symmetry. This means that the buckling geometry effectively lowers the symmetry from the higher D_{6h} point group of planar graphene to the lower D_{3d} point group. This symmetry reduction is directly responsible for many of the unique electronic properties that distinguish stanene from graphene.

3.2. Electronic Properties of Stanene

Stanene consists of a monolayer of tin atoms arranged in a buckled honeycomb structure. Unlike graphene where both sublattices lie in the same plane, stanene has two sublattices that are separated by a small distance along the direction perpendicular to the lattice plane. This vertical separation is precisely the buckling height discussed earlier. To understand the electronic behavior of stanene, one must first examine its

unit cell, Brillouin zone, and the arrangement of nearest neighbor atoms, all of which are illustrated in Figures 3(a) and 3(b).

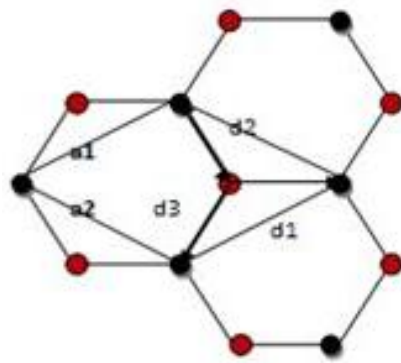
Figure 3(a) shows the primitive unit cell of stanene in real space. The unit cell contains two tin atoms, one from each sublattice, and the lattice vectors a_1 and a_2 define the hexagonal periodicity within the plane. The third lattice vector a_3 points perpendicular to the plane and includes the vacuum spacing necessary for two dimensional calculations. Figure 3(b) displays the corresponding first Brillouin zone in reciprocal space, with the high symmetry points Γ , M, and K clearly marked. These high symmetry points are where the most important electronic features, including the Dirac cones, appear in the band structure.

The lattice vectors for stanene are defined as follows, in agreement with reference [19]:

$$\left. \begin{aligned} a_1 &= a \left(\frac{3}{2}, \frac{\sqrt{3}}{2}, 0 \right) \\ a_2 &= a \left(\frac{3}{2}, -\frac{\sqrt{3}}{2}, 0 \right) \\ a_3 &= a(0, 0, c) \end{aligned} \right\}$$

The reciprocal lattice vectors derived from these are:

$$\left. \begin{aligned} b_1 &= \frac{2\pi}{3a} (1, \sqrt{3}, 0) \\ b_2 &= \frac{2\pi}{3a} (1, -\sqrt{3}, 0) \\ b_3 &= \frac{2\pi}{c} (0, 0, 1) \end{aligned} \right\}$$



(a)

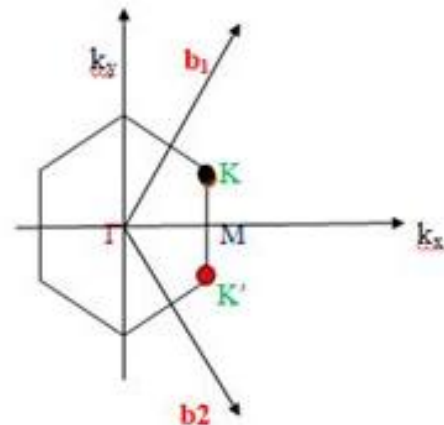
The coordinates of the three nearest neighbor atoms surrounding a given atom on sublattice A are given by:

$$\left. \begin{aligned} d_1 &= (a, 0, \delta) \\ d_2 &= \left(\frac{1}{2}a, \frac{\sqrt{3}}{2}a, \delta \right) \\ d_3 &= \left(\frac{1}{2}a, -\frac{\sqrt{3}}{2}a, \delta \right) \end{aligned} \right\}$$

Here δ represents the buckling height. The high symmetry path used for band structure calculations follows the direction Γ -M-K- Γ , with the coordinates of these points being $\Gamma = (0, 0)$, $M = (2\pi/3a, 0)$, and $K = (2\pi/3a, 2\pi/3\sqrt{3}a)$.

3.2.1. Band Structure of Stanene

The electronic band structure of stanene calculated without spin orbit coupling is presented in Figures 4 (a) and 4 (b). Figure 4 (a) shows the full band dispersion along the high symmetry directions from Γ to M to K and back to Γ . The most striking feature appears near the K point, where the valence and conduction bands meet at a single point. Figure 4 (b) provides a magnified view of the bands around the Fermi level, clearly revealing the linear dispersion characteristic of Dirac cones. These results closely resemble the band structure of graphene and agree well with previously reported calculations [20–22].



(b)

Fig. 3. (a) Primitive unit cell of monolayer stanene showing the lattice vectors a_1 and a_2 within the plane and the two inequivalent tin atoms represented by different colors; (b) First Brillouin zone of the stanene honeycomb structure with high symmetry points Γ , M, and K indicated.

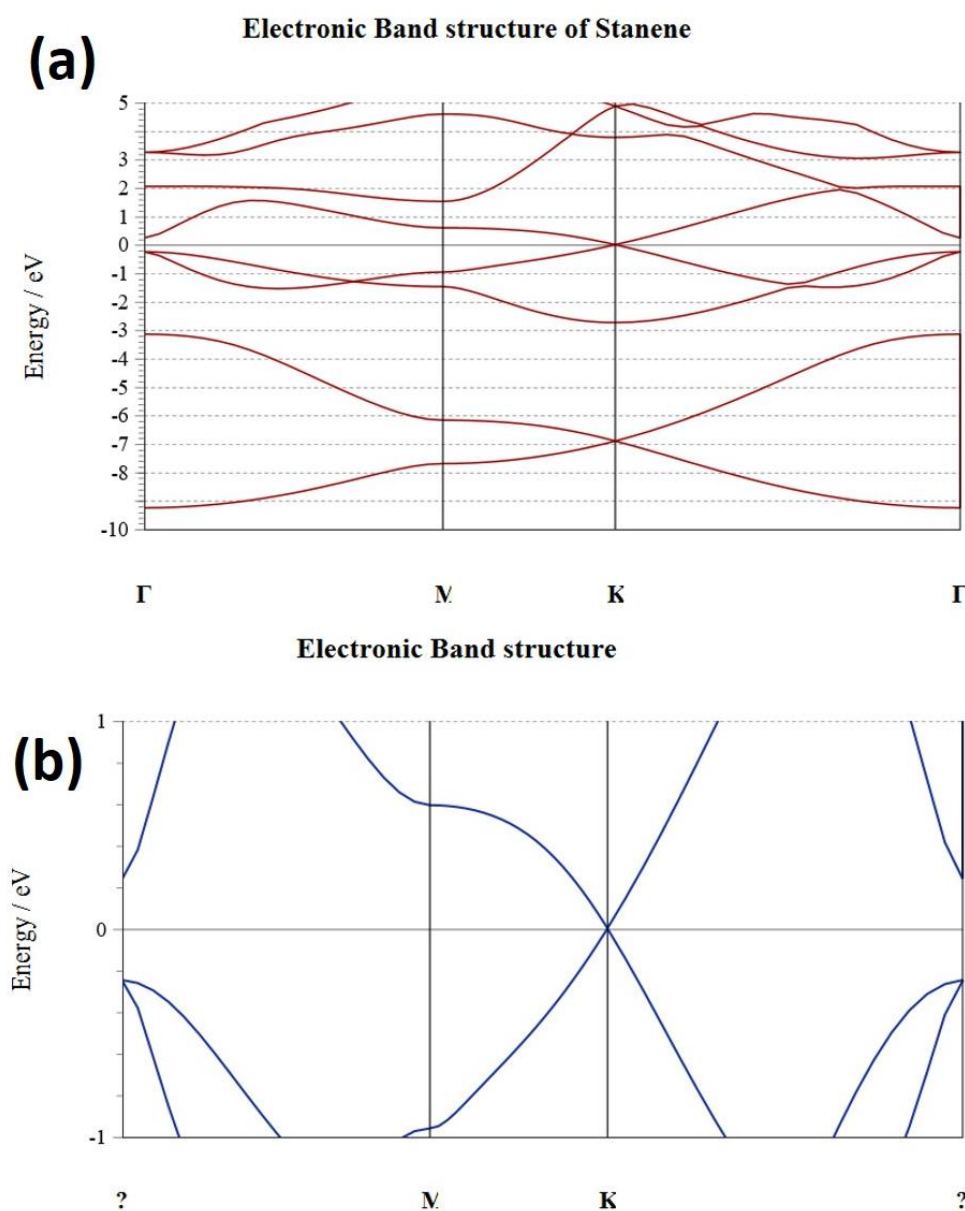


Fig. 4. (a) Electronic band structure of monolayer stanene along the high symmetry directions Γ –M–K– Γ without spin orbit coupling, showing linear crossing at the K point; (b) magnified view of the bands near the Fermi level emphasizing the Dirac cone at the K point.

In free standing, low buckled stanene without spin orbit coupling, linear bands cross exactly at the high symmetry Dirac points K and K'. The electrons near these points obey a relativistic Dirac equation rather than the usual Schrödinger equation, and they behave as massless Dirac fermions. The bottom of the conduction band touches the top of the valence band precisely at the Fermi level, forming a Dirac cone. Consequently, stanene exhibits no band gap and behaves as a zero gap semiconductor or a semimetal. The band structure has a large band gap when spin-orbit (SO) interaction is considered; it behaves as a topological insulator at room temperature and [23].

The band structure of stanene is analogous to that of graphene at Dirac points near Fermi level despite the buckling of stanene structure. The band structure of stanene

differs from that of graphene away from the K or K'. The band structure near the Dirac point for stanene and graphene, highlighting that the linearity in stanene is somewhat reduced compared to graphene. This reduction in linearity arises from the mixed sp^2 – sp^3 hybridization caused by buckling. The energy band gap that opens at the Γ point in stanene is also smaller than that in graphene. When spin orbit coupling is included, a large band gap opens at the Dirac point, and stanene transforms into a topological insulator that could potentially operate at room temperature [23].

3.2.2. Density of States

The total density of states of stanene is shown in Figure 5(a),

and the partial density of states is presented in Figure 5(b). The overall shape of the DOS curve resembles that of graphene, which is expected given their similar band structures. Each tin atom contributes approximately $3.99|e|$ of electronic charge when excluding the d orbital charge, indicating the covalent nature of the Sn–Sn bonds. This value is consistent with previous reports [17, 24].

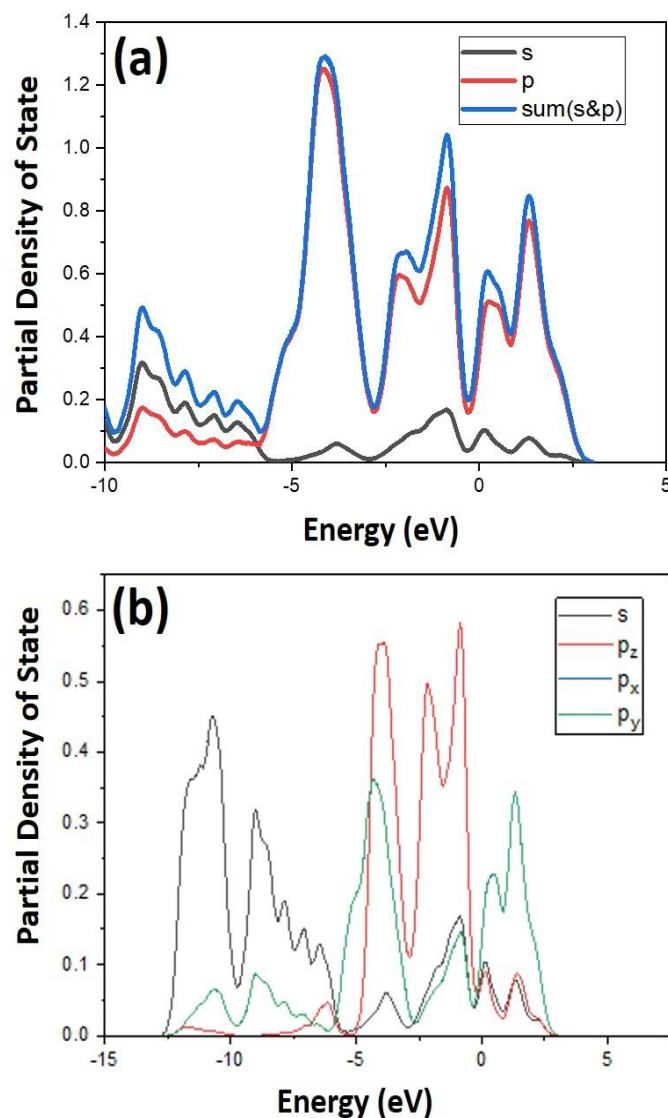


Fig. 5. (a) Total density of states of monolayer stanene as a function of energy relative to the Fermi level, showing vanishing DOS at the Fermi level characteristic of a semimetal; (b) partial density of states showing orbital resolved contributions from s, p_x , p_y , and p_z orbitals, with p_z states dominating near the Fermi level and s states appearing at lower energies.

Examining Figure 5(a), one can see that the density of states at the Fermi level is essentially zero, which confirms the semimetallic character of stanene in the absence of spin orbit coupling. The Fermi level sits exactly at the Dirac point, and there is no gap in the electronic structure. However, the

presence of a finite but very low DOS at the Fermi level distinguishes stanene from true insulators.

Figure 5(b) displays the partial density of states, which separates the contributions from different atomic orbitals. The s and p_z states are found predominantly near the Fermi level due to the mixed sp^2 – sp^3 hybridization. The highly localized nature of electronic states in stanene produces narrow bands in the electronic structure and correspondingly sharp features in the DOS. The PDOS analysis reveals an important orbital specificity. The bands at the K point originate purely from the p_z orbital, meaning that the Dirac fermions are entirely p_z derived. In contrast, the bands at the Γ point result from a combination of p_z orbitals and hybridization between p_{xy} and p_z orbitals, with the conduction band and valence band showing different mixing characteristics [25].

4. CONCLUSION

In this work, we have systematically explored the structural and electronic properties of monolayer stanene using first principles calculations based on density functional theory as implemented in the Quantum ESPRESSO package. The structural optimization clearly shows that stanene prefers a low buckled configuration over a perfectly planar one. This buckling arises from mixed sp^2 – sp^3 hybridization and plays a decisive role in stabilizing the monolayer. The calculated lattice parameters, bond lengths, and buckling height match well with previous theoretical and experimental reports, confirming the reliability of our computational setup. Moving to electronic properties, the band structure of stanene without spin-orbit coupling closely resembles that of graphene. Linear Dirac cones appear at the K and K' points, and the Fermi level passes exactly through these crossing points, indicating a gapless semimetallic state. However, unlike graphene, stanene exhibits reduced linearity at the Dirac point due to the presence of buckling. The density of states analysis further supports this semimetallic picture, with a clear zero gap at the Fermi level. The partial density of states reveals that the p_z orbital dominates the states near the Fermi level, while s and p_{xy} orbitals contribute at deeper energy levels. The most significant finding is the effect of spin-orbit coupling. When SOC is included, a direct band gap opens at the Dirac point, which is absent in the scalar relativistic calculation. This gap opening is a direct consequence of the strong spin orbit interaction in tin, a heavy element. This transformation from a gapless semimetal to a band insulator with nontrivial topology positions stanene as a promising room temperature topological insulator. The magnitude of this band gap can be further tuned by external factors such as electric fields, substrate interactions, or chemical functionalization. In summary, our study confirms that stanene is not merely a heavier analogue of graphene but a distinct material where buckling and spin orbit coupling collectively produce rich and tunable electronic behavior, suitable for future applications in low power electronics and quantum devices.

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

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Availability of data and material

All of the data obtained or analyzed during this study is included in the report that was submitted.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Authors' contributions

All authors contributed equally in the preparation of this manuscript.

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