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PREFACE

Welcome to the 2nd International Science, Engineering and Technology Colloquium 2025 (ISETC 2025)!

It is with great pleasure that we present this year's colloquium, a distinguished gathering of scholars, researchers, and professionals dedicated to the advancement of applied sciences. Held virtually on 9th July 2025, ISETC 2025 serves as a platform to highlight cutting-edge research, foster meaningful networking, encourage collaborations, and explore innovative solutions to global challenges.

This year's theme, "The Power of Scientific Innovation: Intelligent Solutions for a Sustainable World" highlights our shared goal to solve global challenges through applied science. It celebrates innovation as a key to building a more sustainable and resilient future. We're proud to feature keynote speakers and presenters who bring fresh insights, bold ideas, and breakthroughs shaping tomorrow's world.

We would like to extend our heartfelt appreciation to the Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, for their outstanding support and assistance throughout the planning and execution of the event. Their dedication has been instrumental to the success of this colloquium. We would like to sincerely thank all participants and researchers for their valuable contributions. We also appreciate the reviewers for their careful evaluations and helpful feedback. Your hard work and support mean a lot to us.

As editors, we are proud to present this collection of proceedings. It is an honour to bring together the interesting and meaningful work of our speakers and authors. We hope the ideas shared will lead to new discoveries, encourage more research, and help solve global challenges through science and innovation.

Warm regards,

Dr. Emi Norzehan Mohamad Mahbob
Dr. Saiyidah Nafisah Hashim
Ms. Lili Widarti Zainuddin
Ms. Nurul Nazwa Mohammad
Ms. Rozaina Saleh

ISETC 2025 Proceedings Editors

STRUCTURAL AND ELECTRONIC PROPERTIES OF SINGLE LAYER FLAT STANENE: A COMPUTATIONAL STUDY

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Abstract: Stanene, a single-layer arrangement of tin atoms, is considered a two-dimensional (2D) material. This tin analogue of graphene is predicted to be a topological insulator. However, further specific studies are needed to confirm and characterize the electronic properties of this material. Motivated by this, the present work aims to investigate the structural and electronic properties of single-layer flat stanene using a first-principles theoretical framework. In this study, a hexagonal honeycomb structure was constructed and optimized, yielding a lattice constant of 4.2 Å, a bond length of 2.4 Å, and a bond angle of 120˚. The electronic properties of single-layer stanene were then determined. Results show that flat stanene is gapless while preserving a Dirac point along the K path of its band structure, indicating its potential as a topological insulator. Additionally, analysis of the density of states and the charge density distribution suggests that stanene exhibits a hybrid bonding character with both ionic and covalent components. All calculations were carried out using the density functional theory (DFT) framework. A total of 50 electrons per tin atom were considered in the configuration. It is hoped that the findings from this study will be valuable for researchers exploring topological insulator materials for future electronic applications.

***Keywords*:** *Stanene, density functional theory (DFT), band structure, density of states, topological insulator*

INTRODUCTION

The groundbreaking discovery of graphene has significantly shaped the trajectory of materials science, particularly in the field of electronics. Thanks to its outstanding mechanical strength, thermal conductivity, and unique electronic characteristics, graphene has inspired researchers to explore other materials with similar two-dimensional (2D) structures (Yuhara et al., 2018). In an effort to diversify its applications, scientists began modifying graphene—cutting it into nanoribbons, rolling it into nanotubes, or chemically altering its surface—to unlock new functional properties (Mojumder et al., 2015). This study aims to investigate the structure and electronic behavior of single-layer flat stanene using first-principles calculations based on the density functional theory (DFT) framework. By optimizing wavefunction parameters and simulating electronic properties—such as the band structure, density of states, and electron density—this research provides foundational insights for future experimental and device-level studies. The findings may also enhance our understanding of superconductivity in 2D materials, with stanene potentially serving as a substitute for more established systems like graphene or silicene.

MATERIALS AND METHODS

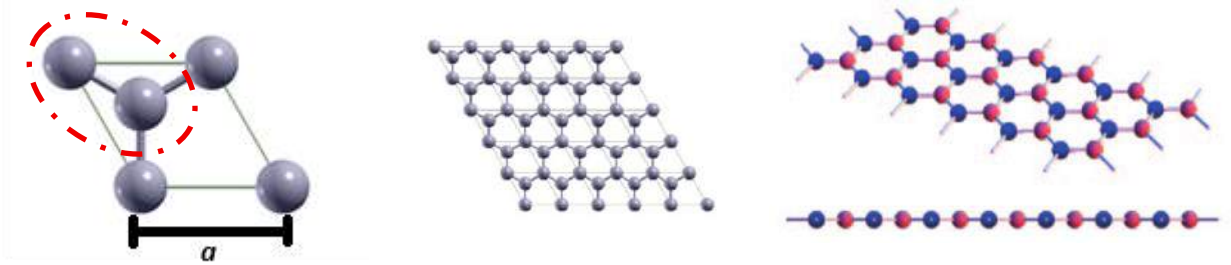
In this research, first part of the simulation requires the density functional theory (DFT) method to perform and compute the data calculations in order to investigate the electronic structure and properties of single layer stanene. Apart of DFT, Quantum Espresso (QE) package with plane wave basis set is used to carry out electronic structure calculations based on self-consistent field solution of Kohn-Sham equation. QE is suitable to use in this project because the scope of study is in repeating unit cell which is in periodic array (Shaidu & Akin-Ojo, 2016). Then, the exchange correlation functional of Perdew, Burke, and Ernzerhof (PBE) (*User's Guide for Quantum ESPRESSO (v.6.6)*, n.d.) under Generalized Gradient Approximation (GGA) scheme worked together with ultrasoft pseudopotential configuration were treated the electron orbital configuration used for calculation of single layer stanene. The initial structure is then sketched and optimized as well as computing its linear combination of atomic orbital for the total electronic structure of the stanene.

In order to obtain correct determination of electronic properties, firstly the optimization step for the cell parameters and atomic coordinates with variable cell relax (vc-relax) are needed. Theoretically, two-dimensional tin has predicted crystallographic data that are calculated at low temperature but non-zero temperature. First, for calculation, we set the DFT configuration to use 0K temperature as to avoid any temperature variability for the system. Then, we let the system to optimize and relaxed the cell parameters, the geometry until it reached lowest energy possible which stand for the most stable, and optimized unit cell. The bravais lattice is set up to 4th mode in QE to indicate that the structure has hexagonal lattice with cell dimensions of 4.6595 and 4.0571 lattice parameters respectively. Type of atom is one with two atoms because the scope of study is a single layer of stanene. The energy cut off of 40.0 Ry had been set-up for wave function and dispersion relation of the plane wave to obtain the electronic structure. For stanene, type of distribution used when smearing is Gaussian. Algorithm of bfgs (Broyden-Fletcher-Goldfarb-Shanno) is specified to optimize the cell parameters. The integration of irreducible Brillouin Zone (BZ) is sampled up to $28 \times 28 \times 1$ k-points for planar system within the Monkhorst-Pack scheme. All atoms in the unit cell are fully optimized when the force in each atom is less than 10^{-8} Ry.

Next, the structure properties are optimized within new cell parameters that obtained from vc-relax calculation. For a difficult geometry optimization which takes more than 50 steps, we increased until 1000 steps. Pseudopotentials file for stanene uses Unified Pseudopotential Format (UPF) extension where it can be found at the Quantum Espresso official portal. Pseudopotentials operator generates the electrons, where 50 electrons for each atom in stanene. Then, it simplifies the atom by dividing the core electron and point charge. The core electrons are excluded through the use of norm-conserving pseudopotentials. Meanwhile, only the point charge or the valence electron takes into consideration by using plane wave with a kinetic energy cut off of 40 eV (Nigam et al., 2015). The projector augmented wave (PAW) method implements with an energy cut off that used to expand the Kohn-Sham wave functions. After relax calculation, self-consistent field (SCF) calculation was carried out. All the optimized and output file that have been visualized using XcrySDen. The study of electronic properties of single layer stanene that consist of band structure, density of states and electron density were calculated throughout the SCF calculation. This calculation is done by approximately solving one particle Schrodinger equation with constant potential. Generally, band structure is calculated with certain k-points that lies on the path that crossed several high symmetry points of the Brillouin zone. In the present case, we chose the point name Gamma (Γ) → X → K → Gamma (Γ) path was chosen. Total of 28 grid k-points were implemented on the pathway of the bandstructure plotting. In order to get fine details of the eigenstates, total 12 band energies for symmetrically divided into each state for conduction and valance bands. Next, the bandstucture were plotted with the help of Python and matplotlib. For the characteristic of the density of states, non-consistent field (nscf) calculation was performed based on the result of self-consistent field calculation from the previous step. The number of k-points mesh were changed to 32. Then, the calculation and occupations are converted into nscf and tetrahedra respectively. Tetrahedra worked together with automatically generated k-points grid to avoid generation of additional k-points in low symmetry case. However, the output data is tedious to plot the graph. Thus, post processing of PWSCF was performed. The simplified data in file is visualized into the graph by using gnuplot package. Post processing in Quantum Espresso were also used to determine the charge density or electron density in a single layer stanene. The raw data was converted into 3D by creating post processing file and the output file of it being visualized by XCrySden for the graphics of the electron density at each atom in the unit cell.

RESULTS AND DISCUSSION

In order to study the structural and electronic properties of single layer stanene, all the data collections were analyzed in graphical method by plotting the graphs, as well as the images. The structure of single layer stanene were constructed and optimized. Meanwhile, the electronic properties such as band structure and density of states (DOS) were plotted into graph and electron density is visualized in the form of picture. Then, the data was compared from the previous study such as graphene, silicene and germanene as the material is in periodic array class. Stanene in group (IV) has the atomic arrangement in a hexagonal honeycomb lattice with two atoms in each primitive cell as shown in Figure 1(a) marked as dashed round with red ink. The structure is similar to another element of planar group (IV) such as graphene, silicene and germanene (Wang et al., 2015). Ezawa (2018) showed the structure of planar graphene (Ezawa et al., 2018). Figure 1(c) proved that group (IV) material has the same type of structure which is hexagonal. Besides, Jomehpour and his co-researchers studied the structure of gemanene also got the hexagonal lattice (Jomehpour Zaveh et al., 2016).



(a) (b) (c)

Figure 1. (a) Structural properties of a single unit cell of Stanene (b) Structural properties of Stanene in periodic array (c) Top view (upper part) and Side view (bottom part) view of Planar Graphene (Ezawa et al., 2018)

The unit cell of stanene contains two Sn atoms with an optimized lattice constant of 4.2 Å as in Figure 1(a). The result is reasonable agreement with the lattice constant reported previously results of 4.67 Å (Abbasi & Sardroodi, 2018). Meanwhile, the lattice constant of graphene, silicene and germanene is 2.45 Å, 3.86 Å and 4.03 Å respectively (Bhuyan et al., 2018). After the relaxation of unit cell, the Sn-Sn bond length was calculated to be $a = 2.4$ Å as shown in Figure 1(a). Abbasi and Sardoodi (2018) concluded the stanene bond length is 2.83 Å. Similar to lattice constant, bond length of stanene is approaching accurate. Apart from that, bond angle of stanene is 120˚ which indicates full sp^3 hybridized due to sp^3 bonding. The result is almost the same with the previous study which is 110˚ (Jiang et al., 2017). To conclude, the optimized crystal structure of single layer stanene resembled a planar hexagonal honeycomb lattice with two primitive atoms in each unit cell same as another element in group IV. After the relaxation, the lattice parameter, bond length and bond angle of stanene are 4.2 Å, 2.4 Å and 120˚ respectively.

Figure 2 represents that stanene is a topological insulator because the conduction band and valence band meet at 0eV where no band gap resulted at the high symmetry points (marked as dashed box with red ink). The band looks like crossing but actually the valence band touches the conduction band at fermi level. Furthermore, the clearly Dirac point shown at the fermi level where the electron transportation from valence to conduction band is accessible. Electrons can move freely without phonon effect. Gapless of forbidden gap shows the properties of semimetal shown by the result from previous study such as graphene from group IV. From the previous study, germanene have zero energy band gap (Jomehpour Zaveh et al., 2016). Result of stanene band structure is valid enough because of the same band gap value and structure with group IV elements. From the result in band structure of stanene, the classification of elements is often revealed where it behaves as semi-metallic and topological insulator. They are able to conduct electricity at the edge of the structure while behave as insulator inside of the elements. Topological insulator behavior even portrays as 100% efficiency where there is no energy loss in conducting electricity because of the single flow.

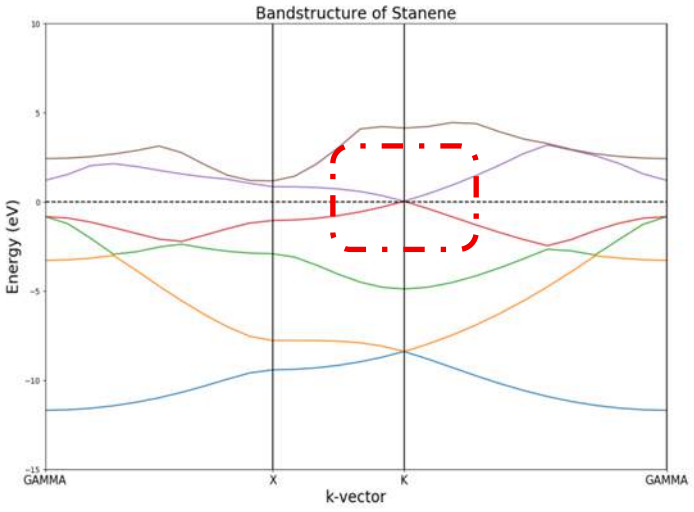


Figure 2. Band Structure of Stanene shows a Dirac Point at K

CONCLUSIONS

In summary, this computational work shows that stanene have hexagonal honeycomb structure with 4.2 Å lattice parameter, 2.4 Å bond length and 120˚ bond angle respectively. It can be said that this work is the same line according to the previous results values close enough from the previous study (Jiang et al., 2017; Mortazavi et al., 2017). An electronic property of hexagonal structure shows that stanene is a good conductor with gapless energy under semi-metal behavior. We found also that stanene is a topological insulator property that acts as conductor at the edge of the material while behave as insulator inside the material. This also can be proven with the obtained bonding type which are ionic and covalent bond from the electron density using plane wave calculation and visualization from XCrySDen. Stanene was also turns to occupy both ionic and covalent bonding characteristics. The uniqueness of the electronic properties of single layer hexagonal honeycomb stanene is able to implicate the applications on the spintronic and photoelectric devices such as sensors which enables to replace other materials that have similar properties such as graphene, germanene and silicene. Also, it may give improvement in the application of superconductor especially as a topology at a 100% efficiency. Future research is recommended to study the multilayer of stanene and optical properties for more accurate data.

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Sekian, terima kasih.

"BERKHIDMAT UNTUK NEGARA"

Setuju.

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SITI BASRIYAH SHAIK BAHARUDIN
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