



# MANY BODY ASPECTS OF LATTICE DYNAMICAL ELASTIC AND THERMAL PROPERTIES OF SILICENE

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## Abstract

Silicene is a two-dimensional material showing high promises for nanoelectronics and thermoelectric applications due to its quantum spin Hall effect and tunable bandgap. However, a complete theoretical understanding of its fundamental properties like thermal and elastic behaviors and its comparison with graphene has remained elusive. This paper investigates the lattice dynamics, thermal conductivity, and elastic constants of Silicene. The calculations show the buckled structure of Silicene couples the out-of-plane flexural vibrations with small in-plane components breaking the planar symmetry existing in graphene. Due to weaker interatomic bonds, the acoustic phonon branches are less dispersive reducing the group velocities and thermal conductivity as compared to graphene where over 80% of heat is conveyed by the ZA flexural branch. The observed value of lattice thermal conductivity of 28.51 W/mK for Silicene agrees well with previous reports. The elastic properties including, Bulk modulus, Young's modulus, Shear modulus, and Poisson's ratio have also been evaluated to assess mechanical stability. The insights developed on the lattice dynamics and thermomechanical characteristics through this comparative assessment deepen the fundamental understanding of two-dimensional crystals for facilitating ongoing explorations focused on device applications of Silicene.

**Keywords:** Silicene, Graphene, Elastic constant, Density functional theory, lattice dynamics, thermal conductivity

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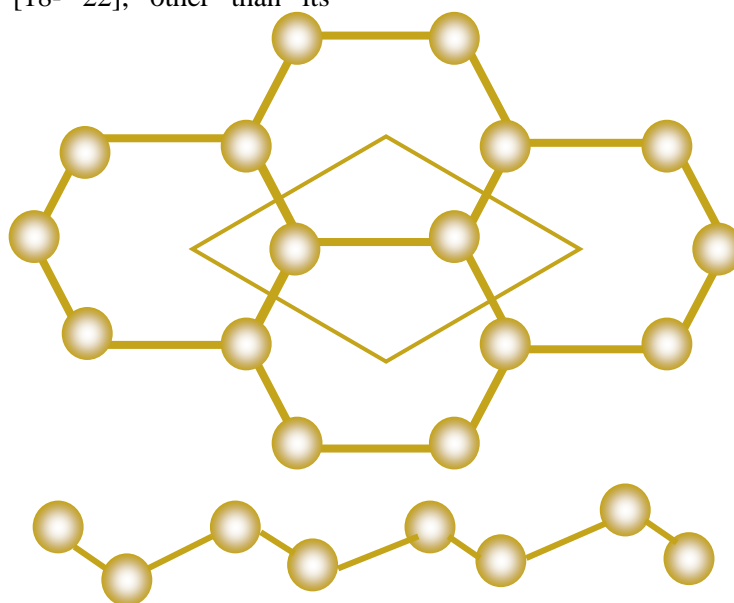
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## 1. Introduction

Two-dimensional (2D) materials are now an emerging area of study in nanomaterials research because of their possible incorporation into next-generation energy conversion and electrical devices [1-4]. Recent developments in graphene and the subsequent discovery of its useful characteristics [5] have led to an increased investigation into comparable two-dimensional systems [6], which includes the study of allotropes of graphene in addition to other two-dimensional materials [7]-[8]. Due to its exceptional material characteristics for a wide range of industrial and basic scientific applications, graphene has drawn a lot of interest since it was discovered [9]-[10]. Experimental and theoretical investigations have shown that graphene has a very high thermal conductivity, between 2000 and 5000 W/mK at normal temperatures [11- 13]. So far, there has been an abundance of studies on the phonon transportation mechanism of graphene [14-17] and its possible uses as an enabling material for thermal management [18- 22], other than its

electronic and optoelectronic uses. However, a consensus on these uses has not been achieved just yet.

In recent years, there has been a significant amount of interest in a wide variety of alternative 2-D materials, such as Silicene and MoS<sub>2</sub>, which are anticipated to contain some of the exceptional features that graphene has, in addition to other distinctive properties that graphene does not possess. This interest has been stimulated by the advancements that have been realized in graphene. For example, Silicene, which is a honeycomb crystal built of silicon (Si) element (as shown in Figure 1) and resembles graphene in two dimensions, represents one of the most promising materials. Over the last year, Silicene has gathered an increasing amount of attention due to the possibility that it is suitable for Si-based systems [23]. This is mostly due to its potential use in semiconductor devices, which are paired with a lattice that is comparable to carbon [23].



**Figure 1. Atomic structure of Silicene [24].**

After its discovery in 1994 theoretical research by Takeda and Shiraishi, it was reinvestigated in 2007 by two scientists who named it Silicene. Silicene, in terms of structure, is a two-dimensional sheet composed of a hexagonal arrangement of Si atoms, that resembles graphene but differs in that the bonds that are bend out-of-plane [25]. The outer layer of Silicene displays ordered swirls and is more reactive with the surfaces of other materials compared to graphene because of chair-like deformation in the rings, which makes it unstable as a completely flat sheet. Therefore, Silicene is an energetically advantageous low-buckled structure because  $sp^3$

hybridization is more stable compared to  $sp^2$  in Si [26]. Theoretically, a vertical electric field should be able to regulate the buckling, which would result in a gap in the band and polarized spin-states [27], which gives Silicene a distinct advantage over graphene. This low buckled structure has been found to be the most stable in previous studies [28].

Graphene and Silicene have very similar electrical characteristics because of their shared lattice arrangements. Similar to graphene, Silicene also has a massless fermion as its charge carrier [29]-[30]. But Silicene's honeycomb lattice is somewhat bent, giving it certain unique properties

that aren't present in graphene's flat form. As an example, a nontrivial difficulty for graphene is the buckled structure, which violates the crystal's symmetry and allows the application of an electric field to open a bandgap [31][32].

From a theoretical perspective, Silicene has exceptional characteristics, but a large-scale practical synthesis of the material is still difficult [33]. The electrical characteristics of Silicene have received a lot of attention, but its thermal, elastic, and lattice properties have received much less attention, despite the fact that these qualities are essential for the performance and dependability of future electronic and optoelectrical devices that make use of Silicene. Exploring and comparing these properties in both 2-D materials is extremely interesting because of the resemblances and variations in lattice structure between graphene and Silicene. This might provide insight into the phonon dispersion of other 2-D materials that display a large range of elastic and thermal properties [34].

The remaining parts of the study are organized in the given way: Section 2 offers a review of research conducted by several authors that examine different characteristics of Silicene. Section 3 outlines the recommended technique for investigating the properties of Silicene in comparison to graphene and includes an evaluation of the methods used. Section 4 provides an in-depth analysis of the outcomes achieved by Silicene across different testing approaches. Finally, Section 6 concludes the overall research, highlighting the potential future areas of development for Silicene.

## 2. Related work

Several studies have been conducted in recent years on Silicene because of its increasing popularity as an emerging material. The findings of several authors are summarized below:

**Routu et al., (2022) [35]** utilized the first principles of density functional theory (DFT) simulations for different hydrogen occupancy on Silicene to study the optical and elastic characteristics of hydrogenated Silicene. Silicene with a hydrogen content of 25% or 75% causes structural asymmetry, which in turn affects the material's optical bandgap and elasticity. The simulation findings of phonon and binding energies revealed that the stability of Silicene increases after hydrogenation.

**Noshin et al., (2021) [36]** investigated Silicene-supported bilayer and hetero-bilayer nanoribbons for semiconductor technology. Molecular dynamics and first-principal calculations revealed around 43% reduction in thermal conductivity for

Silicene/germanene nanoribbons and a 25% reduction for Silicene/graphene nanoribbons compared to pristine Silicene and graphene, respectively. These heterostructures show potential for optimized thermoelectric and enhanced absorption coefficients in the UV region, suggesting applications in optoelectronic devices like UV photodetectors.

**Glavin et al. (2020) [37]** examined elemental two-dimensional materials based on deficiencies and functionality, allotropes, and the links between structure and property. Moreover, the proposed study provided a comprehensive summary of the increasing uses of elemental two-dimensional materials in the fields of electronics, sensing, and other areas, showcasing transformative potential in cutting-edge technologies.

**Zhang et al., (2019) [38]** addressed the challenge of accurately assessing thermal conductivity (TC) in Silicene for Si-based electronic devices. The study introduced a Gaussian approximation potential (GAP) derived from ab initio training data, surpassing other potentials in describing Silicene's properties. Sinusoidal molecular dynamics simulations using GAP revealed a TC of  $32.40 \pm 2.9$  W/mK at room temperature, in strong agreement with Boltzmann transport equation predictions of around 30 W/mK. This underscores the potential of GAP, in predicting TC at the DFT level.

**Hartman et al. (2019) [39]** delved into the issue of the derivatization of group 14 2D materials beyond graphene. Additionally, the study outlined their synthesis techniques and chemical/physical characteristics. It was observed that the band gaps can be changed through surface modification or mono- or few-layered exfoliation which also improves stability. This study discussed the existing trends in this area and gave some insights into possible ways of further development of 2D materials beyond graphene.

**Das et al., (2018) [40]** explored the mechanical properties of Silicene through molecular dynamics (MD) simulations. The study involved various testing methods, including tensile, bending, oscillation, and equilibrium tests. At 298 K the Silicene sheet exhibited plastic flow with a remarkable 46% elongation. The material displayed an ultimate tensile strength of 23.96 GPa, Young's modulus of 5.25 TPa, bulk modulus of 3.62 TPa, yield strength = 18.28 GPa, and cohesive energy of 3.72 eV. This underscores the exceptional mechanical strength of Silicene, positioning it as a potential reinforcing agent.

**Pun et al., (2017) [41]** aimed to develop an optimized interatomic potential for Si using a

modified Tersoff model. They assessed its performance against various Si properties. The proposed potential demonstrated enhanced performance and reasonable agreement with first principles binding energies. Single-layer Silicene was found to be mechanically stable at low temperatures but collapsed at room temperature, while bilayer Silicene exhibited greater stability, suggesting potential existence in a free-standing form at ambient conditions.

**Mortazavi et al., (2017) [42]** employed first-principles DFT to explore the mechanical properties of 2D group-IV allotropes. Uniaxial tensile and compressive simulations revealed insights into stress-strain behavior, including Poisson's ratio ( $\nu$ ) and Young's modulus ( $Y$ ). According to the findings of the study, uniaxial stress might change the electrical nature of buckled structures to a metallic character in every instance, which emphasized the influence of the chirality on the mechanical response of buckling structures. This study contributes a concise

**Rouhi and Saeed et al., (2017) [43]** examine the elastic characteristics of hydrogen-embedded Silicene nanosheets through molecular dynamics simulations. In this study fracture stress and strain along with elastic modulus were calculated to demonstrate that the mechanical properties declined when Silicene was saturated with hydrogen atoms. The results indicated that the armchair type of both zigzag and silicene nanosheets have higher mechanical strength than their zigzag counterparts leading to brittle behaviour. For each type of single-layered material considered in this study, there is an inverse relation between temperature and mechanical properties. This study provides significant findings on the outcome of temperature fluctuations and hydrogen functionalization on the mechanical behavior of monolayered Si-C units.

**Xie et al., (2014) [44]** utilized the first-principal calculation to examine the TC of Silicene. Silicene's phonon transport is not focused properly despite the large number of studies on its electrical characteristics. The study discovered that a monolayer of Silicene has a thermal conductivity of 9.40 W/mK at 300 K, which is significantly smaller compared to bulk silicon. As compared to graphene, out-of-plane vibrations contributed less than 10% to TC and this was due to a small buckling in Silicene causing strong scattering in flexural modes and disruptive reflection symmetry of the material. This study offered significant information on how Silicene thermally behaves and its applications beyond just graphene.

### 3. Methodology

The multiple aspects of lattice dynamical, elastic and thermal properties of Silicene are investigated experimentally in this study. A comprehensive approach has been taken for this purpose. The experimental process involves employing DFT calculations, a first-principal quantum mechanical modeling technique, to investigate the lattice dynamics of Silicene. Lattice thermal conductivity is determined using the Asen-Palmer modified version of Debye-Callaway theory, considering physical models for phonon lifetimes. The elastic properties are assessed by theoretically calculating elastic constants. Additionally, thermal properties, including specific heat, group velocity, average sound velocity, and Debye temperature, are determined through DFT simulations. The entire experimental study integrates modeling and simulation techniques to provide insights into the multifaceted aspects of Silicene's behaviour under different conditions.

#### 3.1 Testing methods

This section presents the testing methods that are used to investigate the various properties of Silicene.

##### 3.1.1 Analysing Lattice dynamics

The lattice dynamical properties of Silicene include analysis of the phonon dispersion relations. Since Silicene and graphene share some similarities and differences in their lattice structures. These structural aspects significantly impact their thermal properties and phonon transport mechanisms. An analysis of the 6 phonon branches present in both materials namely the flexural acoustic (ZA), transverse acoustic (TA), longitudinal acoustic (LA), flexural optical (ZO), transverse optical (TO), and longitudinal optical (LO) branches reveals intriguing insights. In Silicene, the flexural branch has minor in-plane components in contrast to graphene where the flexural mode consists purely of out-of-plane vibrations. Overall, the buckled nature of Silicene's lattice leads to distinguishable thermal conductivity patterns compared to planar graphene. The study analyzed the phonon dispersion of Silicene because phonon dispersion governs lattice dynamics and thermal properties of materials hence it is important to examine.

##### 3.1.2 Evaluation of Thermal Properties

The dependability and efficiency of electrical and optoelectronic devices that use Silicene are significantly affected by its thermal characteristics. Therefore, the thermal conductivity of Silicene has been the subject of a growing amount of research recently [45]. The

thermal conductivity of Silicene has also been the subject of much research. First principles DFT calculations provide the basis of these computations [34]. Computational techniques were used to determine that the inherent thermal conductivity at room temperature is 3-25 W mK<sup>-1</sup> [46][47].

The differences in thermal conductivity of Silicene may be explained through an examination of the phonon Boltzmann transport equation [48]. The equation that describes the thermal conductivity of a material is as follows:

$$\text{Thermal conductivity (K)} = \sum C_p v_p^2 T_p \quad (1)$$

Where  $C_p$ , indicate the heatcapacity,  $v_p$  represents the group velocity, and  $T_p$  is the relaxation time of phonon when all phonon modes  $p$  of a system are taken together.

$$k_i = \frac{1}{3} C_i T^3 \left\{ \int_0^{\theta_i/T} \frac{T_c^i(x) x^4 e^x}{(e^x - 1)^2} dx + \frac{\left[ \int_0^{\theta_i/T} \frac{T_c^i(x) x^4 e^x}{T_N^i (e^x - 1)^2} dx \right]^2}{\int_0^{\theta_i/T} \frac{T_c^i(x) x^4 e^x}{T_N^i T_U^i (e^x - 1)^2} dx} \right\} \quad (2)$$

where  $\theta_i$  is the Debye temperature,  $x = \frac{\hbar\omega}{k_B T}$ ,  $C_i = \left( \frac{k_B^4}{2\pi^2 \hbar^3 v_i} \right)$ ,  $T_c^i$  is the relaxation time.

The variables under consideration are the Boltzmann constant ( $k_B$ ), the Planck constant ( $\hbar$ ), the phonon frequency ( $\omega$ ), and the transverse or longitudinal acoustic phonon velocity ( $v_i$ ).

### 3.1.3 Elasticity Assessment

An in-depth comprehension of the mechanical characteristics is essential for assessing the dependability, robustness, and structural configuration of devices using Silicene. Graphene has significant nonlinear elastic characteristics. This behavior is ubiquitous among various 2D materials with layers, such as graphene, Silicene, stanene, and so on. In the linear theory of elasticity, it is assumed that the deformations are very small. It is enough to consider second and third-order elastic constants to better understand the elastic stress-strain response in these materials. According to Hook's law, the relationship between strain and stress is linear. For extremely small strains, the relationship is as follows:

$$\sigma_i = \sum_j C_{ij} \epsilon_j \quad (3)$$

Where  $C_{ij}$  is elastic stiffness constant that can be calculated as:

$$\epsilon_i = S_{ij} \sigma_j \quad (4)$$

Where  $S_{ij}$  is called elastic compliance constant.

From the above calculation, the various elastic properties can be calculated as follows:

The capacity for transferring heat across a sample with a temperature gradient between its two ends is known as its lattice thermal conductivity (K) [43]. One technique to determine the value of K is by using the relaxation time method to the Debye-Callaway model [44]. The model represents the  $T_p$  as a function of the Debye temperature ( $\Theta$ ), phonon velocity ( $v$ ), and the Grüneisen parameter ( $\gamma$ ), which is caused by the phonon dispersion. A computationally practical methodology to predict the value of K using experimentally observed parameters ( $\Theta$ ,  $v$ , and  $\gamma$ ) is the base of the Debye-Callaway model. In order to determine the value of K of Silicene, the Asen-Palmer modified form of the Debye Callaway formulation is used in this study. In order to determine the value of  $k$  for  $i = \{TA, LA\}$  the following expression is utilized:

$$\text{Young's modulus (Y}_{2D}) = \frac{C_{11}^2 - C_{12}^2}{C_{11}} \quad (5)$$

$$\text{Shear modulus (G)} = \frac{C_{11} - C_{12}}{2} \quad (6)$$

$$\text{bulk modulus (B)} = \frac{C_{11} + C_{12}}{2} \quad (7)$$

$$\text{poisons ratio } (\sigma) = \frac{C_{12}}{C_{11}} \quad (8)$$

Where  $C_{11}$  and  $C_{12}$  are the 2<sup>nd</sup> and 3<sup>rd</sup>-order elastic constants respectively.

## 4. Result and Discussion

This section contains a detailed discussion of the findings that were achieved, which can be found below. Under zigzag uniaxial tension, a critical strain induces a phase transition from the original low-buckle structure to a completely planar hexagonal Silicene, establishing mechanical stability through phonon dispersion analysis.

The failure mechanisms under uniaxial tension—whether along the armchair or zigzag direction—involve elastic instability and subsequent phonon instability. Equiaxial tension, on the other hand, leads to failure solely through elastic instability. An intriguing aspect is the anisotropic behavior of Silicene's Poisson's ratio under strain engineering. The findings of Silicene after using test procedures and making observations are described in the part that follows the mechanical behavior of Silicene, a two-dimensional nanomaterial, is studied in detail under different tension orientations and temperatures using a combination of molecular dynamics (MD) simulations and density functional theory (DFT) calculations.

Interestingly, despite the isotropic Young's modulus for Silicene membranes, the final strain—the highest strain capacity before failure—is shown to be anisotropic, varying between armchair (AC) and zigzag (ZZ) orientations. The optimum strength of Silicene is larger along the

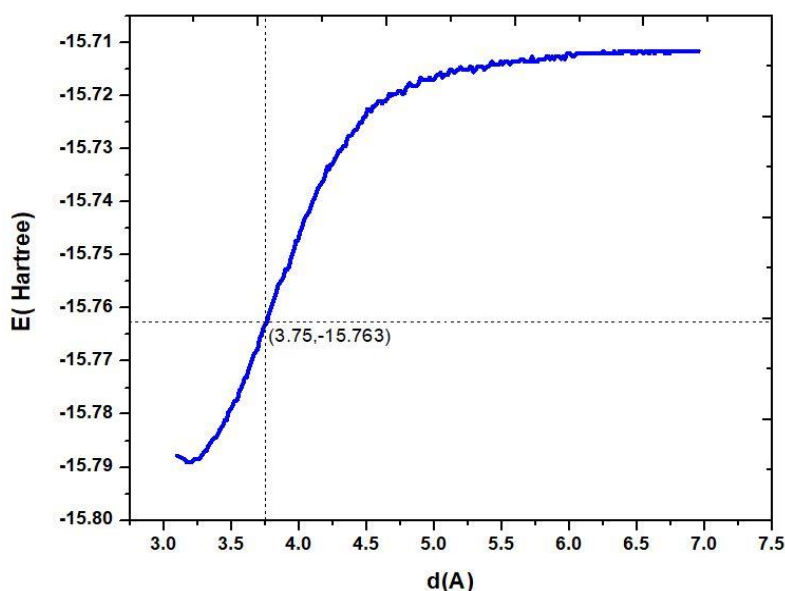
armchair orientation than the zigzag orientation, according to DFT calculations. The theoretical results of ultimate strengths and ultimate strains under armchair (AC), zigzag (ZZ) and equiaxial (EQ) tensions in current work are summarized in Table 1.

**Table 1 shows the ultimate in-plane strengths and stresses of monolayer Silicene under equiaxial (EQ), zigzag (ZZ), and armchair (AC) tensions derived from MD simulations using classical potentials and DFT calculations.**

Material	Ultimate Strength (N.m <sup>-1</sup> )	Ultimate Strength (N.m <sup>-1</sup> )	Ultimate Strength (N.m <sup>-1</sup> )	Ultimate Strain(N/m <sup>2</sup> )	Ultimate Strain(N/m <sup>2</sup> )	Ultimate Strain (N/m <sup>2</sup> )
	AC	ZZ	EQ	AC	ZZ	EQ
Peng (DFT 0 K)	6	5.9	6.2	0.17	0.21	0.17
Zhao (DFT 0 K)	7.07	5.66	-	0.18	0.14	-
Yang (DFT 0 K)	7.39	5.26	6.76	0.17	0.136	0.16
Peri (MEAM 300 K)	3.89	3.94	-	0.18	0.21	-
Roman (ReaxFF 10 K)	4.78	5.85	-	0.089	0.18	-

Stress-strain curves demonstrate a brittle fracture characteristic in Silicene under tension deformation. The absence of apparent plastic deformation before fracture is evident in the abrupt drop in stresses upon reaching the fracture strength. MD simulations further illustrate the fracture process, showing crack nucleation at a critical Si-Si bond breaking point, followed by spontaneous crack propagation leading to a

cleavage failure mode devoid of plasticity. In summary, the comprehensive analysis underscores the anisotropic nature of Silicene mechanical properties, its phase transitions, failure mechanisms, and the significant impact of temperature on its fracture behavior. The optimum breaking point is located at (3.75, -15.763).



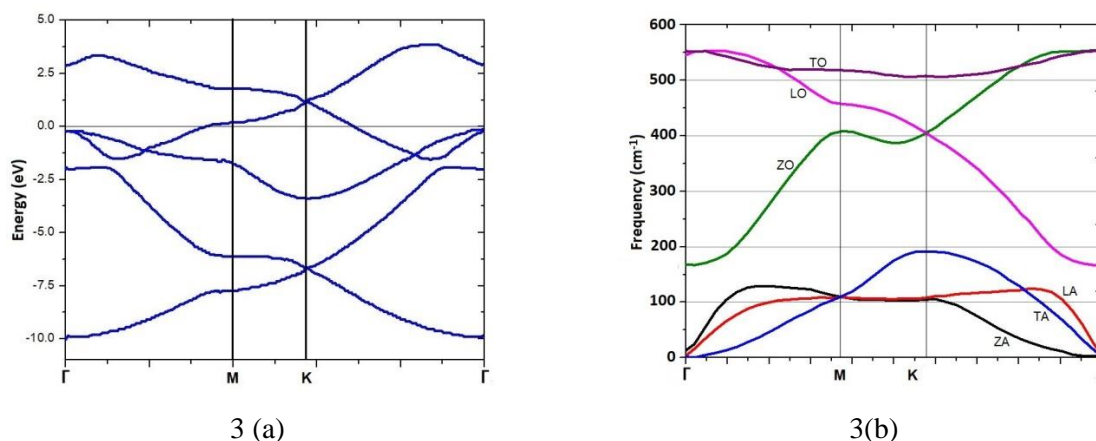
**Figure 2. The silicon lattice's E (hartree) – d (Å) curves showing the transition from three-dimensional to 2D structure evolution. The key position for bond breakdown is indicated by the dashed lines.**

#### 4.1 Phonon dispersion

Figures 3(a) and 3(b) illustrate the electronic band structure of Silicene with low buckling without inclusion of spin-orbit coupling phonon dispersions of Silicene. The flexural mode of Silicene comprises small elements along the in-plane directions, in contrast to the out-of-plane

vibration that occurs in Graphene flexural mode. As a result of the buckling structure of Silicene, the reflectional symmetries over the XY plane have been broken, which, in turn, leads to the coupling of vibration modes that are out-of-plane and in-plane. As a result of its buckling structure, the ZA branches of Silicene have a component

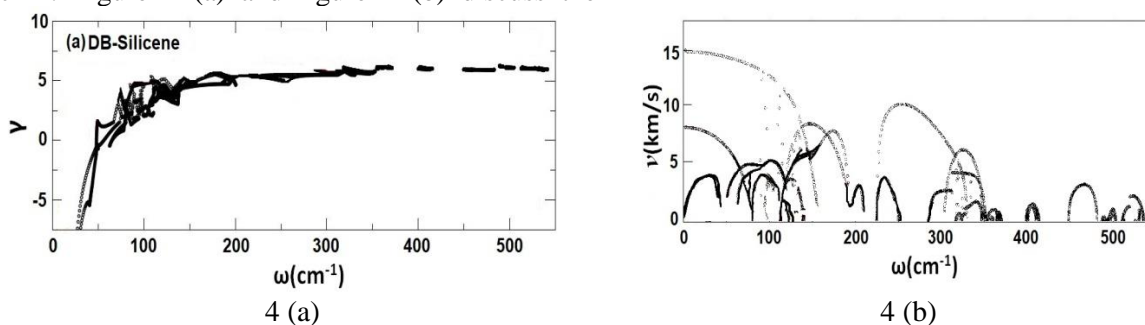
that is linear at the  $\Gamma$  point because of its buckling structure. A low acoustic velocity of 1.01 km/s is the result of this. The LA and TA branches of Silicene are not highly dispersive because the strength of Si–Si bonds is lower than that of C–C bonds. Phonon dispersion in Silicene has low LO oscillations at the  $\Gamma$  point with a frequency of 570  $\text{cm}^{-1}$ .



**Figure 3. Electronic band structure of Silicene with low buckling without inclusion of spin–orbit coupling and Phonon dispersions of Silicene.**

For Silicene, the average sound velocities of the DB-Silicene branches are within 15 Km/s range, whereas, Gruneisen parameter( $\gamma$ ) lies within the range of 5.74 for frequency varying from 0 to 550  $\text{cm}^{-1}$ . Figure 4 (a) and figure 4 (b) discuss the

Gruneisen factor ( $\gamma$ ) and acoustic phonon group velocity ( $v$ ) of DB Silicene, respectively which are compared in relation to their vibration frequency.



**Figure 4: Gruneisen factor ( $\gamma$ ) and acoustic phonon group velocity ( $v$ ) of DB Silicene that are compared in relation to their vibration frequency.**

#### 4.2 Thermal properties

Two acoustic modes—LB and DB—primarily dictate the value of  $k$  because optical branches have a lower acoustic velocity ( $v_p$ ) than acoustic branches. The enharmonic crystalline vibrations, achieved by phonon-phonon scattering, limit the basic phonon transit. It has been demonstrated that Silicene, with its tight similarity index, has a greater phonon dispersion rate than graphene. Silicene has a shorter lifespan because of its higher rate of dispersion, which suggests that more phonons are likely to be scattered. Graphene flexural mode is characterized by vibrations that are completely out of the plane, whereas Silicene's

flexural mode is characterized by the existence of small components along the in-plane directions. The variation arises from the breakdown of the symmetric refraction across the X-Y plane by the buckling framework of Silicene, which leads to the coupling of both in-plane and out-of-plane vibration modes. The acoustic branches (LA and TA) of Silicene are significantly less dispersive than those of Graphene because the Si–Si bonds in Silicene are weaker than those in Graphene. Because to its decreased When comparing the TA and LA modes' scattering rate to that of graphene, the ZA mode accounts for more than 80% of the value of  $K$ . The scattering of the ZA phase in

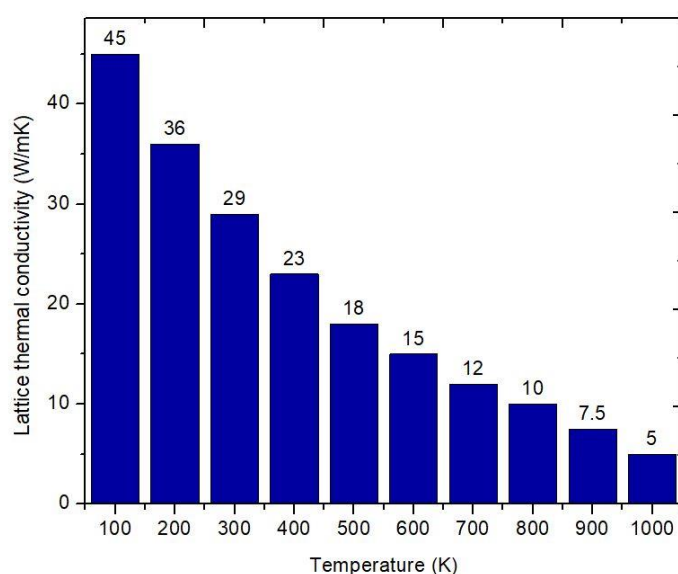
Silicene is equal for both of these modes when compared with LA and TA. According to the Boltzmann transport equation, the ZA mode's ( $v_p$ ) in Silicene is of an order of magnitude smaller than that of the TA and LA modes.

This explains why the ZA mode's influence on the value of K is lowered to less than 10%. This lower Silicene K value is the result of weaker acoustic branches that are less dispersive. This explains why the ZA mode's influence on the value of K has been reduced by less than 10%. Because of the weak Si–Si bonding, there may be less dispersive acoustic branching present, which lowers the value of  $v_p$  and  $T_{pof}$  phonon and contributes to the reduced value of K of Silicene. Alternatively, it can be the consequence of the out-of-plane

coupling and in-plane vibration modes due to the buckling structure, which restricts the heat transmission that the ZA mode facilitates.

#### 4.2.1 Lattice thermal conductivity (K)

The value of K as a function of temperature for Silicene can be observed in Figures 5 respectively. As would be predicted for a phonon-dominated crystalline material, the thermal conductivity falls as the temperature becomes higher. Based on the calculations, the value of K for Silicene is about 5.15 W/mK at 1000 K, whereas for it is 45.1 W/mK at 100 K.



**Figure 5. Lattice thermal conductivity of Silicene**

By taking into consideration the effects that result from transverse acoustic (TA) and longitudinal acoustic (LA) phonon modes, the Debye Callaway formalism—a mathematical framework for understanding thermal conductivity in materials—was employed to evaluate the thermal conductivity of the lattice (k) structure of Silicene, in addition to low buckled (LB) and double buckled (DB) sheets. This technique faces a problem for planar Silicene, as it predicts an implausible increase in the thermal conductivity at the Gamma ( $\Gamma$ )-point as the phonon frequency reaches zero. The formalism includes a buckling altitude of 3.3 Å to deal with this as well as provide a more precise assessment; k is estimated using a value derived from experimental data. This modification is required because the distinct phonon transport characteristics of strictly two-dimensional (2D) materials, such as Silicene, cannot be easily examined using without

assumptions valid for three-dimensional materials, such as bulk graphite.

On the other hand, for LB and DB sheets, the formalism produces results that are in good alignment with empirical and other theoretical data, suggesting that it is useful in forecasting the heat conductivity of these buckling structures. In the context of heat transport modeling, buckling provides a pseudo-third dimensional outcome that enables these materials to be handled more like conventional crystals. In general, DB sheets exhibit lower thermal conductivity than their LB equivalents, with DB Silicene exhibiting the least value among them. The comparison reveals that LB Silicene exhibits a higher thermal conductivity over LB Silicene. This aligns with the hypothesis that, as complexity of structure and phonon scattering chances increase—both of which are more common in DB structures—that thermal conductivity will decrease.



All strictly 2D materials exhibit a temperature-dependent drop in thermal conductivity that is consistent with phonon-dominated transport mechanisms. At higher temperatures, phonon-phonon dispersion becomes more significant and impedes heat transfer. Because 2D materials differ

from an ideal planar geometry, the Debye Callaway approach performs differently across these materials, highlighting the significance of structural subtleties in determining heat transport qualities and emphasizing the need for customized techniques.

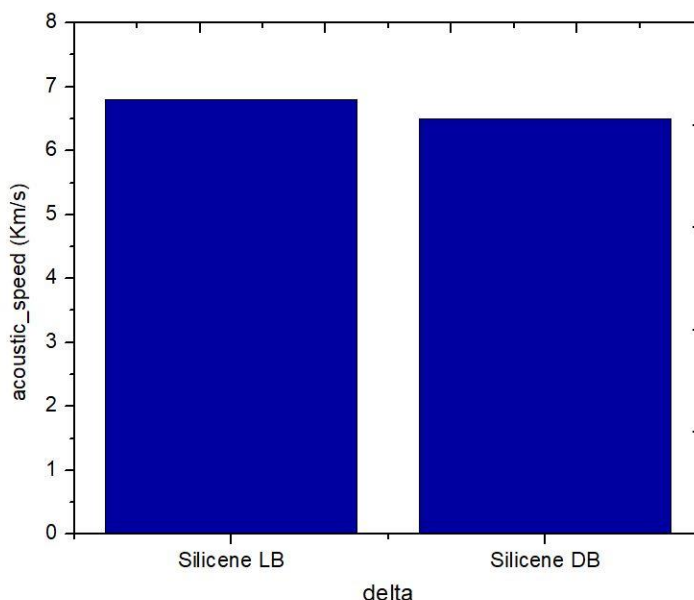


Figure 6. Average acoustic speed of Silicene sample with LB and DB variation.

It is clear from the Figure 6 that Silicene thermal conductivity is reduced by at least a factor of 0.09. This suggests that although the Debye Callaway formalism provides a foundation for comprehending heat transfer in Silicene, which provides its ability to adequately represent the material's high degree of thermal conductivity on the Silicene plane. This disparity seems mostly in

Graphene due to the oversimplification of phonon scattering processes in the DFT band analysis. Figure 7 shows the response of different Silicene unit with Debye temperature (K) variation. It maintains thermal conductivity despite the LB and DB variation.

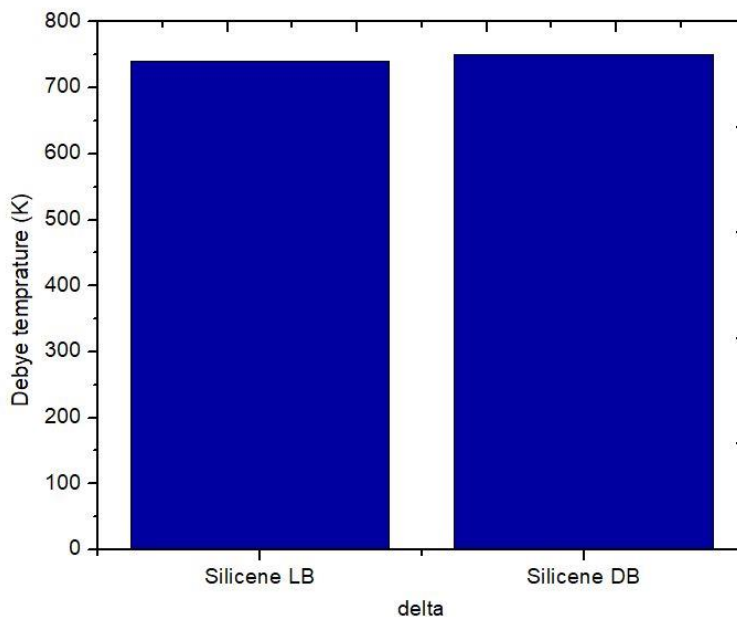


Figure 7. Debye temperature of Silicene sample with LB and DB variation.

In contrast to bulk materials, the intricacies of in-plane vibration driven transport in 2D materials are not adequately addressed by analogously providing a frequency threshold for the Phonon dispersion process.

### 4.3 Elastic properties

Table 2 displays the in-plane Young's modulus ( $E$ ), Poisson's ratio ( $\nu$ ), and second- and third-order elasticity constants for monolayer Silicene derived from DFT calculations. To develop Silicene-based devices and comprehend the practical strength and dependability of these devices, one must have a thorough understanding of Silicene's mechanical properties. The freestanding monolayer graphene showed a significant nonlinear elastic deformation during tensile strain unless the inherent breaking strength capacity (or ultimate strength) is reached, despite the fact that there hasn't been a mechanical experiment on Silicene sheets yet. To put it another way, graphene has nonlinear elastic

characteristics, which may be a common occurrence for other 2D monolayer materials like Silicene.

The second order constants (SOEC) and third-order elastic constants (TOEC) of Silicene have been calculated to characterize both the linear and nonlinear elasticity of Silicene, respectively, using the homogeneous deformation method used in DFT calculations.

Table 2 summarizes the theoretical findings of Silicene from several groups. It is clear that while there are some variations in the TOEC, particularly the  $C_{112}$ , different DFT computations produce almost equal values for the SOEC. Subsequent examination of the strain–energy curves revealed that, at strains greater than around 3.5%, third-order effects became predominant, highlighting the significance of nonlinear elasticity in Silicene.

**Table 2. Second and third order elastic constants in-plane Young's modulus ( $E$ ), Poisson ratio ( $\nu$ ) of monolayer Silicene sheet from DFT calculations All data are in units of Nm except that  $\nu$  is dimensionless.**

Second and third order elastic constants	$c_{11}$	$c_{12}$	$c_{111}$	$c_{112}$	$c_{222}$	$E$	$\nu$
Peng43	71.3	23.2	-397.6	-14.1	-318.9	63.8	0.3225
Xu44	70.6	22.7	-400.5	-13.5	-313.7	63.3	0.32
Zhang46	68.9	23.3	-347.7	-23.1	-270.1	61	0.33

Silicene is substantially softer than graphene ( $E = 334$  N/m,  $m = 0.18$ ), having only 20% of the in-plane stiffness and over twice the Poisson's ratio. In general, a material is deemed brittle if its  $\sigma$  value is equal to or less than 0.26; otherwise, it is deemed ductile. The results show that the  $B/G$  and  $\sigma$  values are below their critical values, indicating that Silicene is not brittle at room temperature. It is generally accepted that for elastic and stable materials, the value of  $\sigma$  should be less than 0.5.

Silicene is ductile and stable since the calculated values of  $\sigma$  are less than its critical value.

The values of the Silicene elastic constants determined at room temperature are shown in Table 3, which is provided below. Silicene has less value for  $B$ ,  $Y$ , and  $G$  than graphene. In comparison to graphene  $B/G$ , Silicene has a lower bonding strength and stiffness. Its ' $\sigma$ ' value indicates whether the material is brittle or ductile.

**Table 3. Elastic properties of Silicene**

Material	$M$ (amu)	$Y_{2D}$	$B$	$G$	$\sigma$
Silicene	28.09	63.01	47.61	24.25	0.337

Several important factors that emphasize the special qualities of Silicene as 2D material are detailed in the analysis of its mechanical properties. Based on the weight of a single silicon atom inside the structure, the atomic mass ( $M$ ) of Silicene, which is 28.09amu, provides a fundamental knowledge of its composition. Young's modulus ( $Y_{2D}$ ), a crucial measure, is stated to be 63.01GPa, indicating the considerable

stiffness of Silicene and its resistance to deform under applied stress. In applications where materials with excellent structural integrity are required, this is an important consideration. Silicene's bulk modulus ( $B$ ), which is 47.61GPa, highlights the material's resistance to compressive forces and suggests that robustness is necessary for materials that may be subjected to constant pressure in future uses. The shear modulus ( $G$ )

value of 24.25GPa sheds light on Silicene's rigidity against shearing forces, a measure of how the material distorts under such conditions without changing volume. Lastly, the Poisson's ratio ( $\sigma$ ) of Silicene is reported as 0.337, falling within the expected range for solids, which illustrates its tendency to expand or contract perpendicularly to the direction of stress applied, an important characteristic in understanding the material's behaviour under load. Together, these parameters create a comprehensive picture of Silicene mechanical and thermal performance, underpinning its potential for innovative applications in nanotechnology and materials science.

### 5. Conclusion and Future Scope

To sum up, this work combines sophisticated computational and theoretical methods with a rigorous experimental technique to investigate the structural dynamic, thermal, and elastic features of Silicene in detail. Using Density Functional Theory (DFT) simulations, an essential component of first-principles quantum mechanical modelling, the study carefully investigates the lattice dynamics characteristic of Silicene. The study uses the Asen-Palmer modified formulation of the Debye-Callaway theory, involving precise physical models for measuring phonon lifetimes—a crucial component in comprehending thermal transport mechanisms—to accurately calculate the lattice thermal conductivity. Elastic properties of Silicene are evaluated by theoretically determining its elastic constants, which provide a full understanding of its mechanical strength and deformation response. Additionally, the research explores the thermal properties of Silicene, including Energy, phonon group velocities, average sound velocity, and Debye temperature, all determined via DFT simulations. Consequently, Silicene has a lower thermal conductivity of 28.51 W/mK than graphene with 3846.1 W/mK. Since over 80% of heat is carried by the ZA mode in graphene its contribution reduces below 10% in Silicene. Based on the calculations, the value of K for Silicene is about 5.15 W/mK at 1000 K, whereas for it is 45.1 W/mK at 100 K. The coupling between out-of-plane and in-plane modes and the lower phonon group velocities increases thermal transport in silicene. This holistic experimental approach, combining both modelling and simulation, unveils intricate insights into Silicene's multifaceted behaviour, highlighting its distinctive lattice dynamics and thermal and mechanical

characteristics under varied conditions. The findings underscore the complex interplay between atomic structure and material properties in two-dimensional materials, enriching the understanding of Silicene's potential applications in fields ranging from nanoelectronic to thermoelectric, and setting a precedent for future research in the domain of novel two-dimensional materials.

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