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Many Body Aspects on the Lattice Vibrational Properties of Germanene and Silicene along Highly Symmetry Directions

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ABSTRACT

The investigation of lattice vibrational properties in monolayer two-dimensional honeycomb lattices comprising 2D group-IV semiconductor materials such as Germanene and Silicene (Low Buckled structure) holds immense significance in the realm of research, owing to their potential integration into the forthcoming electronic sector for information technology. The ductile nature of 2D group-IV semiconductor materials enables seamless integration with existing semiconductor technology on substrates, setting them apart from Graphene. Our primary objective revolves around comprehending the lattice vibrational properties of Germanene and Silicene (LB) through the examination of their honeycomb and buckled lattice structures. We use the Adiabatic Bond Charge Model with a Python program to derive vibrational frequencies at the Γ points along highly symmetrical directions. Moreover, we extensively analyze the acoustical and optical contributions to the lattice vibrational frequencies. We anticipate that the phonon frequencies along the *Γ–M* direction for 2D atomically thin Germanene and Silicene will yield reasonably similar outcomes to those other research groups achieve.

Keywords: Adiabatic Bond Charge Model, Lattice Vibrational frequencies, Germanene and Silicene.

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INTRODUCTION

The discovery of Germanene and Silicene (LB), atomically thin, 2D group-IV semiconductor materials, including other materials with honeycomb and buckled lattice structures, has been accomplished.[1-2] The application of Adiabatic Bond Charge models in studying the lattice vibrational properties of 2D group-IV semiconductor materials offers a comprehensive and straightforward explanation of phonon dispersion curves across the entire Brillouin zone (BZ), with clear physical components and minimal computational complexity. Lattice vibrations are responsible for the prominent physico-thermal properties of solids. Within a solid, atoms oscillate around their equilibrium positions. These oscillations, known as lattice vibrations, are influenced by interatomic interactions within the crystal. To determine lattice vibrational frequencies and associated modes, eigenvalues and eigenvectors of the dynamical matrix derived from the interatomic interaction potentials,[7-10] need to be calculated. Once the dynamical matrix is known, solving the eigenvalue problem becomes straightforward. Several theoretical approaches have been employed to understand the lattice vibration properties of Germanene and Silicene.[11-13] These approaches typically involve the force constant model, rigid ion model, rigid shell model, dipole approximation, and others. However, the bond charge model has shown best results for IVth group semiconductors. The ABCM method was originally proposed by Weber.[3] More recently, some research groups have investigated the stable honeycomb structures of Graphene and Silicene, Germanene, and other 2D atomically thin group-IV materials.[4, 5]

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The total energy per unit cell of honeycomb and low buckled structure is

$$\Phi_{total} = 3\left[\phi_i(t)+\phi_1(r_1)+\phi_2(r_2)\right]-\alpha^{eff}{}_M\frac{(3Z)^2e^2}{\varepsilon t}+3\left[V_b^1+V_b^2+\psi_1\left(r^1{}_b\right)+\psi_2\left(r^2{}_b\right)\right]+\frac{1}{2}\hbar\omega_j(q) \quad \ldots\ldots(1)$$

The condition for the non-trival solutions for wave equation (1) lead to the characteristic or secular equation,

$$\left|D^{eff}(q)-\omega^2(q)mIn\right|=0 \quad \ldots\ldots(2)$$

$$\omega=\omega_j(q);\ j=1,2,3,\ldots..2n$$

This is the secular equation of 2x2 dimensions.

$$-\omega^2 m_1 U = [D(0,0) - +D(0,1)D(1,1)^{-1}D(1,0)]U \quad \ldots\ldots(3)$$

where

$$D(0,0) = \begin{pmatrix} D_{xx}(0,0) & D_{xy}(0,0) \\ D_{yx}(0,0) & D_{yy}(0,0) \end{pmatrix} \quad \ldots\ldots(4)$$

$$D(1,0) = \begin{pmatrix} D_{xx}(1,0) & D_{xy}(1,0) \\ D_{yx}(1,0) & D_{yy}(1,0) \end{pmatrix} \quad \ldots\ldots(5)$$

$$D(0,1) = \begin{pmatrix} D_{xx}(0,1) & D_{xy}(0,1) \\ D_{vx}(0,1) & D_{vv}(0,1) \end{pmatrix} \quad \ldots\ldots(6)$$

$$D(1,1) = \begin{pmatrix} D_{xx}(1,1) & D_{xy}(1,1) \\ D_{yx}(1,1) & D_{yy}(1,1) \end{pmatrix} \quad \ldots\ldots(7)$$

The dynamical matrix is

$$D_{\alpha\beta}\left(\frac{kk'}{q}\right) = \sum_{l'} \Phi_{\alpha\beta}(l' - l; kk') exp\,(iq.r(lk, l'k') \quad \ldots\ldots(8)$$

The result is investigated along hexagonal Brillouin zone with symmetry points Γ (0,0), M ($\frac{2\pi}{a\sqrt{3}}$,0). The vibrational frequencies along symmetry line with coupling constant γj =0.49 for Germanene and Silicene is deduced as

For *Γ–M,*

$$\omega_1^2 = \gamma_j\left[1 - \cos\left(\frac{\sqrt{3}}{2} q_y a\right)\right] \quad \ldots.(9)$$

$$\omega_2^2 = 3\,\gamma_j\left[1 - \cos\left(\frac{\sqrt{3}}{2} q_y a\right)\right] \quad \ldots.(10)$$

$$\omega_3^2 = \left[\frac{3}{2}\,\gamma_j - \left(\frac{5}{4}\right)\gamma_j - \gamma_j \cos\left(\frac{\sqrt{3}}{2} q_x a\right)\right] \quad \ldots.(11)$$

$$\omega_4^2 = \left[\frac{3}{2}\,\gamma_j + \left(\frac{5}{4}\right)\gamma_j + \gamma_j \cos\left(\frac{\sqrt{3}}{2} q_x a\right)\right] \quad \ldots.(12)$$

$$\omega_5^2 = 0 \quad \ldots.(13)$$

$$\omega_6^2 = 3\,\gamma_j \quad \ldots.(14)$$

PHONON DISPERSION CURVE OF GERMANENE AND SILICENE (LOW BUCKLED STRUCTURE)

Using the phonon dispersion curve at a = 4.06 Å, we computed the different modes as shown in Table 1 with help of Python Program (Appendix - A)

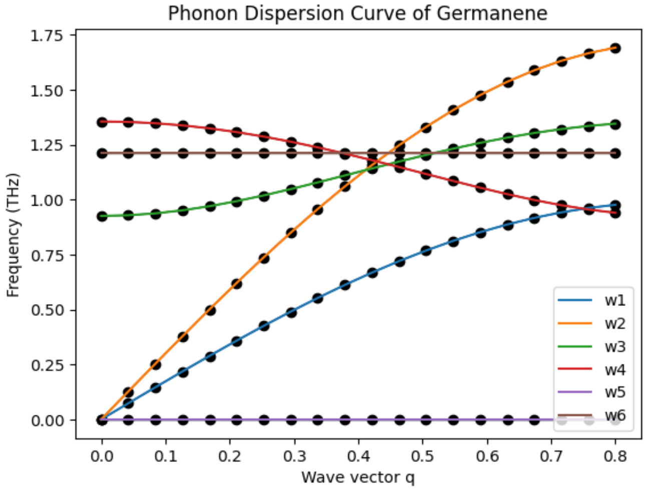

Figure 1: Phonon Dispersion Curve along the highly symmetry directions *Γ-M* for Germanene (LB)

Appendix - A

Table 1: Calculated phonon frequencies (THz) for Germanene (LB)

Wave vector (q)	*Transverse Acoustic mode TA(THz)*	*Longitudi-nal Acoustic mode LA(THz)*	*Z-Direction-Acoustic mode ZA(THz)*	*Longitudinal-Optical mode LO(THz)*	*Transverse -Optical mode TO(THz)*	*Z-Direction-Optical mode ZO(THz)*
0.00	0.000000	0.000000	0.926012	1.355544	0	1.212435
0.04	0.073211	0.126806	0.928902	1.353565	0	1.212435
0.08	0.146022	0.252917	0.937455	1.347656	0	1.212435
0.12	0.218032	0.377644	0.951335	1.337894	0	1.212435
0.16	0.288849	0.500302	0.970017	1.324411	0	1.212435
0.20	0.358084	0.620220	0.992836	1.307392	0	1.212435
0.24	0.425357	0.736741	1.019033	1.287078	0	1.212435
0.28	0.490301	0.849227	1.047805	1.263765	0	1.212435
0.32	0.552560	0.957062	1.078342	1.237811	0	1.212435
0.36	0.611792	1.059656	1.109860	1.209631	0	1.212435
0.40	0.667674	1.156446	1.141616	1.179707	0	1.212435
0.44	0.719899	1.246902	1.172925	1.148583	0	1.212435
0.48	0.768181	1.330529	1.203163	1.116869	0	1.212435
0.52	0.812256	1.406870	1.231771	1.085236	0	1.212435
0.56	0.851883	1.475505	1.258254	1.054416	0	1.212435
0.60	0.886844	1.536059	1.282182	1.025186	0	1.212435
0.64	0.916947	1.588200	1.303185	0.998351	0	1.212435
0.68	0.942029	1.631643	1.320954	0.974720	0	1.212435
0.72	0.961952	1.666150	1.335234	0.955064	0	1.212435
0.76	0.976606	1.691531	1.345830	0.940074	0	1.212435

Appendix - B

Table 2: Calculated phonon frequencies (THz) for Silicene (LB)

Wave vector (q)	*Transverse-Acoustic mode TA(THz)*	*Longitudinal -Acoustic mode LA(THz)*	*Z-Direction-Acoustic mode ZA(THz)*	*Longitudinal-Optical mode LO(THz)*	*Transverse -Optical mode TO(THz)*	*Z-Direction-Optical mode ZO(THz)*
0.00	0.000000	0.000000	0.926012	1.355544	0	1.212435
0.04	0.069791	0.120881	0.928639	1.353746	0	1.212435
0.08	0.139235	0.241162	0.936422	1.348374	0	1.212435
0.12	0.207986	0.360242	0.949082	1.339493	0	1.212435
0.16	0.275702	0.477529	0.966184	1.327210	0	1.212435
0.20	0.342045	0.592441	0.987165	1.311680	0	1.212435
0.24	0.406687	0.704403	1.011382	1.293099	0	1.212435
0.28	0.469305	0.812861	1.038146	1.271712	0	1.212435
0.32	0.529588	0.917273	1.066753	1.247812	0	1.212435
0.36	0.587235	1.017121	1.096515	1.221742	0	1.212435
0.40	0.641960	1.111907	1.126770	1.193895	0	1.212435
0.44	0.693490	1.201160	1.156904	1.164719	0	1.212435
0.48	0.741569	1.284435	1.186349	1.134713	0	1.212435
0.52	0.785957	1.361318	1.214590	1.104432	0	1.212435
0.56	0.826435	1.431427	1.241166	1.074478	0	1.212435
0.60	0.862799	1.494413	1.265671	1.045502	0	1.212435
0.64	0.894870	1.549962	1.287747	1.018187	0	1.212435
0.68	0.922488	1.597797	1.307090	0.993234	0	1.212435
0.72	0.945515	1.637681	1.323442	0.971339	0	1.212435
0.76	0.963837	1.669416	1.336593	0.953161	0	1.212435

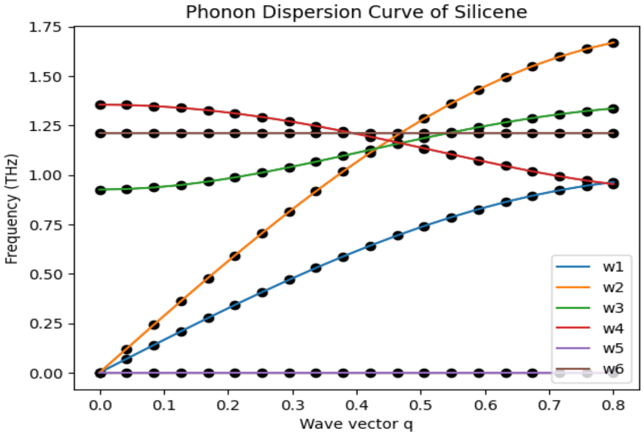

Figure 2: Phonon Dispersion Curve along the highly symmetry directions *Γ-M* for Silicene (LB)

Using the phonon dispersion curve at a = 3.87 Å, we computed the different mode as shown in Table 2 with help of Python Program (Appendix - B)

RESULTS AND DISCUSSION

The computation of lattice vibrational frequencies involved solving the secular equation for the six vibrational frequencies corresponding to phonon wave vectors (q) along the highly symmetry direction *Γ–M*. The lattice vibrational frequencies (ω) were plotted against the wave vector (q) using a Python program to obtain the phonon dispersion curves. The analysis of these curves revealed several important points regarding the phonon dispersion of Germanene and Silicene (LB) along the highly symmetry directions. The longitudinal phonon dispersion exhibited oscillatory behavior in the higher q region, while the transverse phonon curves showed less significant oscillatory behavior for higher q values. This suggests that transverse phonons undergo greater thermal motion compared to longitudinal phonons. The ω-q curves for longitudinal phonons reached their maxima at higher q values. Figure 1 & 2 illustrates the computed phonon dispersion curves of Germanene and Silicene, which aligns with previous work.[15-17] Similar to other 2D atomically thin IVth semiconductor materials, the linear behavior of the longitudinal acoustic (LA) and transverse acoustic (TA) branches near the Γ point was observed.[14] Three-body interactions had a more pronounced impact on LO and TO branches compared to the acoustic branches LA and TA in this group IVth semiconductor 2D materials. For wave vectors along the Γ (0,0) and *M* ($\frac{2\pi}{\alpha\sqrt{3}}$,0) symmetry directions. Three regions of the dispersion curves merit particular attention due to the larger slope of phonon branches in the phonon spectrum. Interestingly, several points in the phonon dispersion curve are noteworthy in Germanene. Several points coincide at the points of inflexion. The LA/LO/TO/ZA phonon modes intersect at 1.22 THz, while the TO/TA phonon modes saturate at 0.939 THz, and the TO phonon mode crosses the LA/ZA phonon modes at 1.188 THz, 1.57

THz and the LA/ZA phonon modes meet at 1.125 THz. The LO/TO phonon modes exhibit small splitting. Similar curves have been observed in Silicene. The LA/LO/TO/ZA phonon modes intersect at 1.188 THz, while the TO/TA phonon modes saturate at 0.939 THz, and the TO phonon mode crosses the LA/ZA phonon modes at 1.157 THz, 1.125 THz and the LA/ZA phonon modes meet at 1.063 THz, showing very strong degeneracy and the LO/TO phonon mode also exhibits small splitting. The dispersion curves along the symmetry line indicate that all six branches are non-degenerate at the Γ (0, 0) and M () points. It is possible to separate LO modes from TO modes in high-symmetry situations. The main characteristic of the dispersion curve is the separation of optic and acoustic mode frequencies across the range of wave vectors, which is attributed to the association of optical vibrations with electric moments. The transverse modes also exhibit a separation of optic and acoustic modes.

Conclusion

This paper presents a systematic report on the phonon dispersion curves along highly symmetry directions of Germanene and Silicene (LB). Based on the overall satisfactory agreement, we conclude that our model, which incorporates three types of interactions: (i) Coulomb interactions, (ii) short-range central force interactions, and (iii) a rotationally invariant Keating-type bond bending interaction dependent on angle, adequately describes the lattice vibrational properties of 2D Group-IV semiconductor materials.[15-18] The incorporation of van der Waals interactions (vWI)[5] has a significant influence on both the longitudinal and transverse optic modes compared to the acoustic branches. Furthermore, the agreement between our theoretical model and experimental data at the Γ point is excellent. Another noteworthy feature of our model is its ability to accurately reproduce almost all branches of the phonon dispersion curves. In this paper, we compare the lattice vibrational properties of Germanene and Silicene (LB) with those reported by other groups of researchers. The theoretical predictions for the vibrational frequencies of Germanene and Silicene (LB) show reasonably good agreement with previous studies.[19- 21]

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References

[1] A. C. Ferrari, F. Bonaccorso, V. Fal'Ko, K. S. Novoselov, S. Roche, P. Bøggild, S. Borini, F. H. Koppens,V. Palermo, N. Pugno, and et al., Nanoscale 7, 4598 (2015).

[2] K. S. Novoselov, V. I. Fal'ko, L. Colombo, P. R. Gellert, M. G. Schwab, and K. Kim, Nature 490, 192 (2012).

[3] W. Weber, Adiabatic bond charge model for phonons in diamond, Si, Ge and α- Sn Phys. Rev. B15, 4789 (1977).

[4] K.C Rustagi and Weber, adiabatic bond charge model for phonons in A3B5 Semiconductors, Sol. Stat.-comm. 18,673 (1976).

[5] M.I.Aziz, Ph.D Thesis, V.B.S.P.U, Jaunpur (2010).

[6] R.K.Singh, Physics Reports (Netherland) 85, 259, (1982).

[7] A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, Theory of Lattice Dynamics in the Harmonic Approximation, Solid State Physics, Vol. 3, Eds. H. Ehrenreich, F. Seitz, and D. Turnbull, Academic Press, New York (1971).

[8] P. BruÈesch, Phonons: Theory and Experiments I (Lattice Dynamics and Models of Interatomic Forces), Springer Ser. Solid State Sci. Vol. 34, Eds. M. Cardona, P. Fulde, and H.-J.Queisser, Springer-Verlag, Berlin/Heidelberg/New York (1982).

[9] Hepplestone S P and Srivastava G P , Lattice dynamics of ultrasmall silicon nanostructures Appl. Phys. Lett.87 231906,(2005).

[10] Hepplestone S P and Srivastava G P , Lattice dynamics of silicon nanostructures, Nanotechnology, 17 ,3288–98, (2006).

[11] Seymur Cahangirov,Hasan Sahin,Guy Le Lay and Angel Rubio Introduction to the Physics of Silicene and other 2D Materials,Springer,(2016).

[12] M. Maniraj, B. Stadtmüller, D. Jungkenn, M. Düvel, S. Emmerich, W. Shi, J. Stöckl, L. Lyu, J. Kollamana, Z. Wei, A. Jurenkow, S. Jakobs, B. Yan, S. Steil, M. Cinchetti, S. Mathias & M. Aeschlimann, Communications Physics , 2, Article number: 12 (2019).

[13] Sumit Saxena, Raghvendra Pratap Chaudhary & Shobha Shukla Scientific Reports, 6, 31073 (2016).

[14] Gour P. Dasa , Parul R. Raghuvanshi, Amrita Bhattacharya, 9th International Conference on Materials Structure and Micromechanics of Fracture Phonons and lattice thermal conductivities of graphene family ,23,334-341, (2019).

[15] Md. Habibur Rahman, Md Shahriar Islam, Md Saniul Islam, Emdadul Haque Chowdhury, Pritom Bose, Rahul Jayan and Md Mahbubul Islam , Physical Chemistry Chemical Physics,23, 11028-11038, (2021).

[16] Novel Lattice Thermal Transport in 2D group-IV materials Bo Peng ,Hao Zhang ,Hezhu Shao , Yuchen Xu , Xiangchao Zhang and Heyuan Zhu, Scientific Reports ,August (2015).

[17] Wu, Liyuan Lu, Pengfei Bi, Jingyun Yang, Chuanghua Song, Yuxin Guan, Pengfei Wang, Shumin,Nanoscale Research Letters,volume 11,525,(2016).

[18] Bo Peng, Hao Zhang, Hezhu Shao,Yuanfeng Xu, Gang Ni, Rongjun Zhang, and Heyuan Zhu,Phys. Rev. B 94, 245420 ,(2016).

[19] Bo Peng, Hao Zhang, Hezhu Shao, Yuchen Xu, Xiangchao Zhang, and Heyuan Zhu, Sci Rep. , 6, 20225, (2016).

[20] Kamlesh Kumar, M. Imran Aziz, American journal of nanosciences,8-12 (2022).

[21] u-Jin Ge, Kai-Lun Yao, and Jing-Tao Lü ,Phys. Rev. B 94, 165433 (2016).

APPENDEX - A

Python Program Of Germanene Along High Symmetry Directions

```
import matplotlib.pyplot as plt
import numpy as np
import math
# #vj = gamma
a = 4.06
vj =0.49
points = np.array([0.00, 0.05, 0.10, 0.15, 0.20, 0.25,0.30,0.35,
0.40, 0.45,0.50,0.55, 0.60, 0.65, 0.70, 0.75, 0.80 ])
```

```
points= np.linspace(0.0,0.8,20)
def solve(fun):
op = []
for qy in points:
op.append(fun(qy))
def ws1f(qy):
return (math.sqrt(vj*(1-math.cos((math.sqrt(3)*qy*a)/2))))
def ws2f(qy):
return (math.sqrt(3*vj*(1-math.cos((math.sqrt(3)*qy*a)/2))))
def ws3f(qx):
return (math.sqrt(((3/2)*vj) + ((5/4)*vj) - (vj*math.cos((math.sqrt(3)*qx*a)/2))))
def ws4f(qx):
return (math.sqrt(((3*vj)/2) + ((5/4)*vj) + vj*math.cos((math.sqrt(3)*qx*a)/2)))
def ws5f(qx):
return 0

def ws6f(qx):
return (math.sqrt(3*vj))
ws1 = solve(ws1f)
ws2 = solve(ws2f)
ws3 = solve(ws3f)
ws4 = solve(ws4f)
ws5 = solve(ws5f)
ws6 = solve(ws6f)
plt.plot(points, ws1, color='k', linewidth = 1,  marker = 'o')
plt.plot(points, ws2, color='k', linewidth = 1,  marker = 'o')
plt.plot(points, ws3, color='k', linewidth = 1,  marker = 'o')
plt.plot(points, ws4, color='k', linewidth = 1,  marker = 'o')
plt.plot(points, ws5, color='k', linewidth = 1,  marker = 'o')
plt.plot(points, ws6, color='k', linewidth = 1,  marker = 'o')
plt.plot(points, ws1, label='w1')
plt.xlabel("Wave vector q")
plt.ylabel("Frequency (THz)")
plt.title("Phonon Dispersion Curve of Germanene")
print (ws1)
# Show the plot
#plt.show()
plt.plot(points, ws2, label='w2')
plt.xlabel("Wave vector q")
plt.ylabel("Frequency (THz)")
plt.title("Phonon Dispersion Curve of Germanene")
print (ws2)
# Show the plot
#plt.show()
plt.plot(points, ws3, label='w3')
plt.xlabel("Wave vector q")
plt.ylabel("Frequency (THz)")
plt.title("Phonon Dispersion Curve of Germanene")
print (ws3)
# Show the plot
#plt.show()
plt.plot(points, ws4, label='w4')
plt.xlabel("Wave vector q")
plt.ylabel("Frequency (THz)")
plt.title("Phonon Dispersion Curve of Germanene")
print (ws4)
# Show the plot
#plt.show()
plt.plot(points, ws5, label='w5')
plt.xlabel("Wave vector q")
plt.ylabel("Frequency (THz)")
plt.title("Phonon Dispersion Curve of Germanene")
print (ws5)
# Show the plot
#plt.show()
plt.plot(points, ws6, label='w6')
plt.xlabel("Wave vector q")
plt.ylabel("Frequency (THz)")
plt.title("Phonon Dispersion Curve of Germanene")
print (ws6)
# Show the plot
plt.legend()
plt.show()
# show the plot
plt.show()
```

APPENDEX - B

Python Program Of Silicene Along High Symmetry Directions

```
Import matplotlib.pyplot as plt
import numpy as np
import math
# #vj = gamma
a = 3.87
vj =0.49
points = np.array([0.00, 0.05, 0.10, 0.15, 0.20, 0.25,0.30,0.35, 0.40, 0.45,0.50,0.55, 0.60, 0.65, 0.70, 0.75, 0.80 ])
points= np.linspace(0.0,0.8,20)
def solve(fun):
op = []
for qy in points:
op.append(fun(qy))
def ws1f(qy):
return (math.sqrt(vj*(1-math.cos((math.sqrt(3)*qy*a)/2))))
def ws2f(qy):
return (math.sqrt(3*vj*(1-math.cos((math.sqrt(3)*qy*a)/2))))
def ws3f(qx):
return (math.sqrt(((3/2)*vj) + ((5/4)*vj) - (vj*math.cos((math.sqrt(3)*qx*a)/2))))
def ws4f(qx):
return (math.sqrt(((3*vj)/2) + ((5/4)*vj) + vj*math.cos((math.sqrt(3)*qx*a)/2)))
def ws5f(qx):
return 0
def ws6f(qx):
```

```
return (math.sqrt(3*vj))
ws1 = solve(ws1f)
ws2 = solve(ws2f)
ws3 = solve(ws3f)
ws4 = solve(ws4f)
ws5 = solve(ws5f)
ws6 = solve(ws6f)
plt.plot(points, ws1, color=’k’, linewidth = 1,  marker = ‘o’)
plt.plot(points, ws2, color=’k’, linewidth = 1,  marker = ‘o’)
plt.plot(points, ws3, color=’k’, linewidth = 1,  marker = ‘o’)
plt.plot(points, ws4, color=’k’, linewidth = 1,  marker = ‘o’)
plt.plot(points, ws5, color=’k’, linewidth = 1,  marker = ‘o’)
plt.plot(points, ws6, color=’k’, linewidth = 1,  marker = ‘o’)
plt.plot(points, ws1, label=’w1’)
plt.xlabel(“Wave vector q”)
plt.ylabel(“Frequency (THz)”)
plt.title(“Phonon Dispersion Curve of Silicene”)
print (ws1)
# Show the plot
#plt.show()
plt.plot(points, ws2, label=’w2’)
plt.xlabel(“Wave vector q”)
plt.ylabel(“Frequency (THz)”)
plt.title(“Phonon Dispersion Curve of Silicene”)
print (ws2)
# Show the plot
#plt.show()
plt.plot(points, ws3, label=’w3’)
plt.xlabel(“Wave vector q”)
plt.ylabel(“Frequency (THz)”)
plt.title(“Phonon Dispersion Curve of Silicene”)
print (ws3)
# Show the plot
#plt.show()
plt.plot(points, ws4, label=’w4’)
plt.xlabel(“Wave vector q”)
plt.ylabel(“Frequency (THz)”)
plt.title(“Phonon Dispersion Curve of Silicene”)
print (ws4)
# Show the plot
#plt.show()
plt.plot(points, ws5, label=’w5’)
plt.xlabel(“Wave vector q”)
plt.ylabel(“Frequency (THz)”)
plt.title(“Phonon Dispersion Curve of Silicene”)
print (ws5)
# Show the plot
#plt.show()
plt.plot(points, ws6, label=’w6’)
plt.xlabel(“Wave vector q”)
plt.ylabel(“Frequency (THz)”)
plt.title(“Phonon Dispersion Curve of Silicene”)
print (ws6)
# Show the plot
plt.legend()
plt.show()
# show the plot
plt.show()
```