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A Theoretical Framework of Mechanical Properties of the Monolayer Graphene

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Abstract: For decades, scientists and researchers believed that two-dimensional (2D) crystals are thermodynamically unstable. Graphene was the first two dimensional material that has successfully been exfoliated from bulk graphite in 2004. We derive interatomic potentials for Graphene for two dimensional lattice structure and using Quasi-harmonic approximations, Mechanical Properties of monolayer Graphene were investigated. The compressibility, hardness, ductility, toughness, brittleness and bonding nature of the Graphene are too well connected with the SOECs. Thus, comprehensive studies on elastic properties are important to show the potential of Graphene in engineering applications. Present studies of monolayer Graphene have been carried out to investigate the elastic constants such as Young's modulus, Poisson's ratio, bulk modulus and shear modulus. With the help of elastic constants, the values longitudinal and transverse sound velocities have been computed. We, at present also find the phonon group velocities at Γ points along symmetry directions by PYTHON Program. Mechanical Properties were calculated by PYTHON program is agreed very close with the result of other researchers.

Keywords: Quasi-Harmonic Approximations, Hamiltonian Mechanics, Elastic Constants, Graphene

1. Introduction

The elasticity is a fundamental property of crystalline solids and is of great importance in physical science, including materials science and solid state physics. The elasticity of materials is concern with the cohesion of solids. In this regard, elastic constants are important parameters for construction of interatomic potentials, the mechanical stability of crystal and wave propagation in two dimensional lattice structures. The Graphene structure has interesting features which is the good reason for studying its Mechanical properties. Graphene is a mono layer of hexagonally arranged carbon atoms which has become practically available today [1-3].

The atoms in the 2D monolayer Graphene are capable of executing oscillations about their equilibrium position (n, l). In oscillating states the instantaneous position of atoms $(n, l))$ is denoted by $r(n, l) = x(n, l) + u(n, l)$.

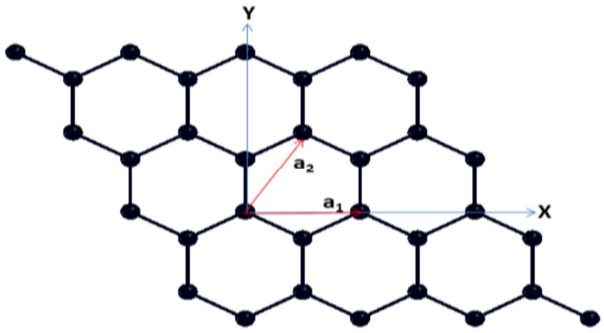

Figure 1. *Structure of Graphene Sheet.*

Thus the Hamiltonian of the Graphene is

$$H = \sum_{nli} \frac{M_n}{2} \dot{u}_i^{\,2}(n,l) + \frac{1}{2} \sum_{nli} \Phi_{ij} \binom{m\ n}{l, l'} \sum_{ml'j} u_i(n,l) u_j(m,l') \quad (1)$$

$$\text{Where } \Phi_{ij} \binom{m\ n}{l, l'} = \left[\frac{\partial^2 U}{\partial u_i(n,l) \partial u_j(m,l')} \right]_0 \quad (2)$$

The notations used here are usual, that is M_n is the mass of

the n^{th} atom, $u_i(n,l)$ is a small displacement of the n^{th} atom in the l^{th} cell along i^{th} direction i, j represent components of Cartesian coordinate axes and U is the ion-ion interaction potential. The force constants are defined as

$\Phi_{ij}\binom{m\ n}{l,l'} = -\gamma\, e_i e_j$, where e_i & e_j are unit vectors, it is the force acting on the n^{th} atom in the l^{th} cell along i^{th} direction due to a unit displacement of the m^{th} atom in the l'^{th} cell along j^{th} direction.

The equation of vibrating motion is given by

$$M_n \ddot{u}_i(n,l) = -\sum_{ml'j} \Phi_{ij}\binom{m\ n}{l,l'} u_j(m,l') \quad (3)$$

The solution of above equation is modified by the periodicity of lattice thus a wave–like solution of type

$$u_i(n,l) = M_n^{-\frac{1}{2}}\, u_{in} exp[i\{q.r(n,l) - \omega(q)t\}] \quad (4)$$

Where u_{in} is the amplitude of vibration along with direction of the n^{th} atom, ω is the angular frequency, q is wave vector, the factor $M_n^{-\frac{1}{2}}$ has been chosen for convenience in further calculation [4, 6, 8].

2. Elastic Modulus of Monolayer Graphene

In the linear theory of elasticity, the infinitesimal deformations are assumed, and second-order elastic constants (SOEC) are sufficient to describe the elastic stress-strain response and wave propagation in solids. For very small strain according to Hook's law strain in linear with stress, give the relation

$$\sigma_i = \sum_j c_{ij}\, \epsilon_j \quad (5)$$

Where c_{ij} are elastic stiffness constantsr

$$\in_i = s_{ij}\sigma_j$$

S_{ij} is called elastic compliance constant

C_{ij} are the forth rank tensor matrices

Graphene has C_{6v} symmetry while Graphene has D_{3d} symmetry, C_{ij} matrices for Graphene and Graphene is given

$$c_g = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2(c_{11}-c_{12}) \end{bmatrix}$$

$$c_s = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & 1/2(c_{11}-c_{12}) \end{bmatrix}$$

2D materials z tends to zero these matrices are same and have only two Elastics constants c_{11} and c_{12}. Hexagonal crystals have the feature that the waves are isotropic in basal plane (q_z =0) that is not true for cubic crystal.

$$c = \begin{bmatrix} c_{11} & c_{12} & 0 \\ c_{12} & c_{11} & 0 \\ 0 & 0 & 1/2(c_{11}-c_{12}) \end{bmatrix}$$

Elastic compliance constants matrix is inverse of elastic stiffness constants matrix i.e

$$s = c^{-1}$$

$$s = \begin{bmatrix} \frac{c_{11}}{c^2{}_{11} - c^2{}_{12}} & \frac{-c_{12}}{c^2{}_{11} - c^2{}_{12}} & 0 \\ \frac{-c_{12}}{c^2{}_{11} - c^2{}_{12}} & \frac{c_{11}}{c^2{}_{11} - c^2{}_{12}} & 0 \\ 0 & 0 & \frac{2}{c_{11}-c_{12}} \end{bmatrix}$$

$$s = \begin{bmatrix} s_{11} & s_{12} & 0 \\ s_{12} & s_{11} & 0 \\ 0 & 0 & 2(s_{11}-s_{12}) \end{bmatrix}$$

Young s modulus

$$E = \frac{1}{s_{11}} = \frac{c^2{}_{11} - c^2{}_{12}}{c_{11}}\ \upsilon = \frac{-s_{12}}{s_{11}} = \frac{c_{12}}{c_{11}}\ s_{66} = 2(s_{11}-s_{12})$$

Shear modulus is inverse of s_{66} i.e

$$G = \frac{1}{s_{66}} = \frac{c_{11}-c_{12}}{2} \quad (6)$$

Bulk modulus of 2D materials that is equivalent to in-plane stiffness constant

The elastic energy density U is a quadratic function of the strains.

$$U = \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2} c_{ij}\, e_i e_j$$

For isotropic e1=e2=1/2δ this give

$$U = \left(\frac{c_{11}+c_{12}}{2}\right)\delta^2$$

$$\text{B}=\left(\frac{c_{11}+c_{12}}{2}\right) \quad (7)$$

Table 1. *Calculated and Compared Young's modulus Y2D, Poisson's ratio σ, bulk modulus B and shear modulus G for Graphene.*

Materials	M (amu)	ρ_{2d} (x10^{-6} Kg/m^2)	Y_{2D} (N/m)	B_{2D}(N/m)	G_{2D} (N/m)	σ
Graphene	12.01	0.7550	340.8020	207.2041	144.6320	0.1802

Table 1 shows the Young's modulus Y_{2D}, Poisson's ratio υ, bulk modulus B and shear modulus G for Graphene estimated at room temperature. It is found that the value of B, Y, and G of Graphene are smaller than Graphene [7, 15, 16]. Thus Graphene have little Stiffness and bonding with respect to Graphene B/G and 'σ' are the measure of brittleness and

ductility of solid. If $\sigma \leq 0.26$ and the solid is generally brittle, otherwise it is ductile in nature. Our finding of lower values of B/G and σ compared to their critical values indicates that Graphene is not brittle in nature at room temperature. It is well known that for stable and elastic material the value of σ should be less than 0.5. The values of 'σ' evaluated for Graphene are smaller than its critical value. The agreement between the calculated elastic constants of the Graphene lattice structure and the experimental values is reasonably good.

3. Longitudinal &Transverse Velocities of Monolayer Graphene

The equation of elasticity is derived from Newton's law:

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \sum_j \frac{\partial^2 \sigma_{ij}}{\partial x_j{}^2} \tag{8}$$

Where ρ_{2d} is surface mass density in units of Kilogram per area.

A sound wave has a displacement given by

$$u(r) = u_0 exp[i(q.r - \omega t)] \tag{9}$$

Time derivative give –iω, and space derivative $\frac{\partial y}{\partial x} \rightarrow iq$. The strains are

$$e_1 = iq_x u_x,\ e_2 = iq_y u_y,\ e_6 = i(q_x u_y + q_y u_x)$$

then equation of motion become

$$(c_{11}{q_x}^2 + \frac{(c_{11}-c_{12})}{2}{q_y}^2 - \rho\omega^2)u_x + \left((c_{11} + \frac{(c_{11}-c_{12})}{2}\right) q_x q_y u_y = 0$$

$$(c_{11}{q_y}^2 + \frac{(c_{11}-c_{12})}{2}{q_x}^2 - \rho\omega^2)u_y + \left((c_{11} + \frac{(c_{11}-c_{12})}{2}\right) q_x q_y u_x = 0$$

It has solution only if the determinant of coefficient of u_x and u_y should be vanishes I $\begin{vmatrix} (c_{11}{q_x}^2 + \frac{(c_{11}-c_{12})}{2}{q_y}^2 - \rho\omega^2) & \left((c_{11} + \frac{(c_{11}-c_{12})}{2}\right) q_x q_y \\ \left((c_{11} + \frac{(c_{11}-c_{12})}{2}\right) q_x q_y & (c_{11}{q_y}^2 + \frac{(c_{11}-c_{12})}{2}{q_x}^2 - \rho\omega^2) \end{vmatrix} = 0.$

Simplify this we obtain

$$\rho^2\omega^4 - \rho\omega^2(c_{11} + \left(\frac{c_{11}-c_{12}}{2}\right)q^2 + c_{11}\frac{(c_{11}-c_{12})}{2}q^4 = 0 \tag{10}$$

This is quadratic equation of $\rho\omega^2$ and its solutions have two values give the longitudinal and transverse acoustic velocities.

$$V_{LA} = \sqrt{\frac{c_{11}}{\rho}} \tag{11}$$

$$V_{TA} = \sqrt{\frac{c_{11}-c_{12}}{2\rho}} \tag{12}$$

Table 2. *Longitudinal and Transverse velocities.*

Materials	Longitudinal velocity (Km/Sec)	Transverse velocity (Km/Sec)
Graphene	21.5903	13.8210

Table 2 shows the variation of Longitudinal &Transverse velocities of monolayer Graphene. It is clear that Longitudinal &Transverse velocities are decreasing for Graphene in comparison to Graphene [9, 10]. It is understandable that the variation of Longitudinal &Transverse velocities is affected by the Phonon group velocities. It may be determined that the average sound wave velocity is a maximum when a sound wave travels with the z-axis of the material.

4. Phonon Group Velocity

The speed of propagation of an acoustic phonon, which is also the speed of sound in the lattice, is given by the slope of the acoustic dispersion relation, $\partial\omega_j/\partial q_j$ i.e.

$$v_g = \frac{d\omega_j}{dq_j} \tag{13}$$

$$q_j = q_x, q_x$$

$$v_{s1} = \frac{\sqrt{3}}{4}a(\gamma_j)^{\frac{1}{2}}\left[\cos\left(\frac{\sqrt{3}}{4}q_y a\right)\right]$$

$$v_{s2} = a\left(\frac{9}{8}\gamma_j\right)^{\frac{1}{2}}\left[\cos\left(\frac{\sqrt{3}}{4}q_y a\right)\right]$$

$$v_{s3} = \frac{\sqrt{3}}{2}a(\gamma_j)^{\frac{1}{2}}\left[\sin\ \left(\frac{\sqrt{3}}{2}q_x a\right) + \sin\ \left(\sqrt{3}q_x a\right)\right]$$

$$v_{s4} = 0$$

$$v_{s5} = 0$$

$$v_{s6} = -\frac{\sqrt{3}}{2}a(11\,\gamma_j)^{\frac{1}{2}}\left[\sin\ \left(\frac{\sqrt{3}}{2}q_x a\right) - \sin\ \left(\sqrt{3}q_x a\right)\right] \quad (14)$$

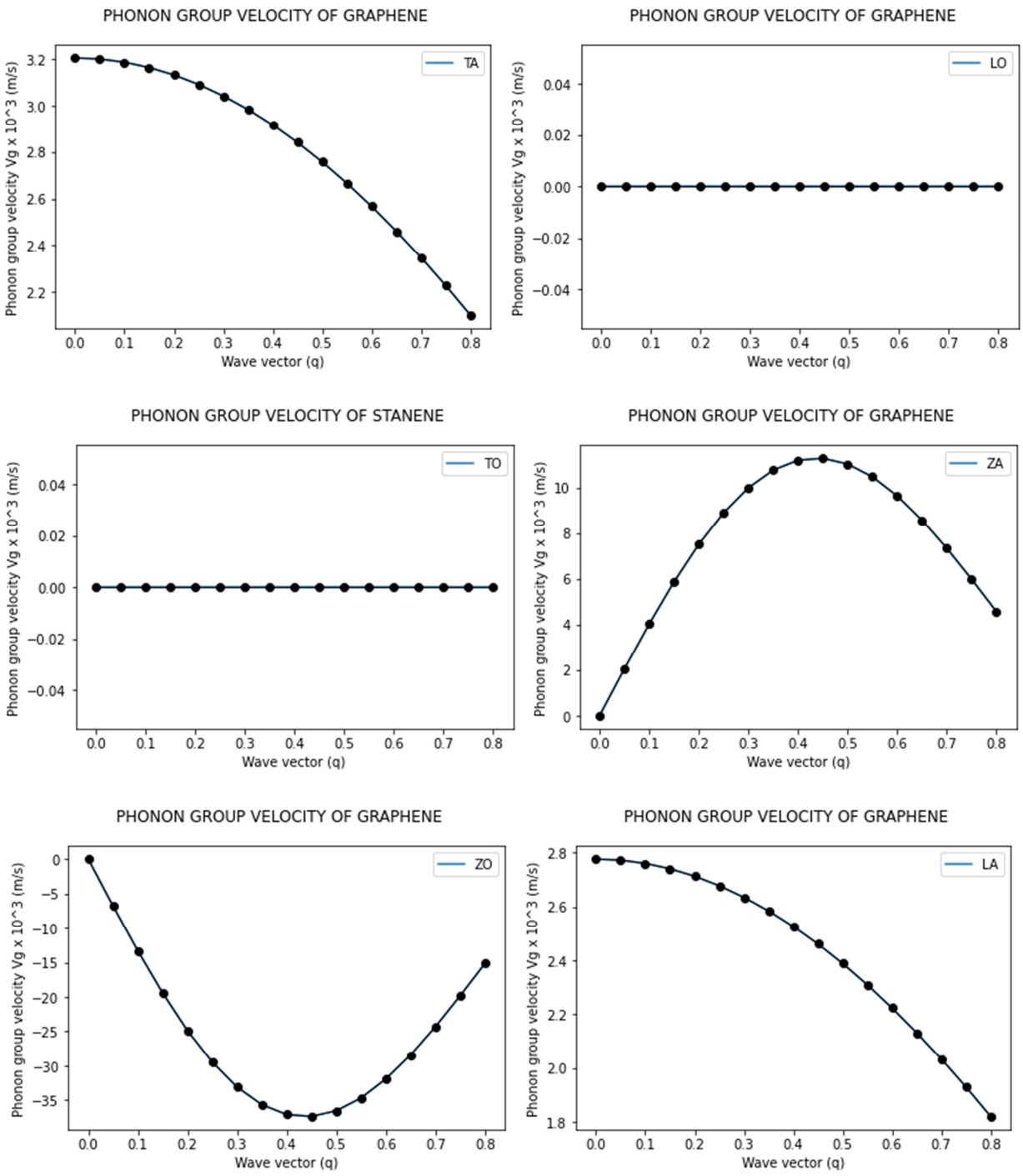

Figure 2. *Calculated Phonon group velocities for Graphene along symmetry line Γ- M.*

The phonon group velocities have been computed by solving the secular equation [12, 13] for the six vibration frequencies corresponding to the phonon wave vectors along the principal symmetry direction *Γ- M* with the help of Python Program. There exists number of phonon branches such as LA, TA, ZA, LO, TO, ZO in Graphene [11] Their existence can be explained by the quantization of lattice waves along the X-Y axis due to partial or complete phonon spatial confinement along the cross-plane direction. Figure 2 shows the group velocities for Graphene. The observations inferred from this figure are as follows, six curves show the group velocity corresponding to six phonon branches. The group velocity has been reduced in the nanostructure due to complete phonon confinement. Group velocity approaches to zero as wave vector approaches to zero. Some phonon branches have more group velocity as compared to bulk. No

phonon branch has velocity more than that in bulk cladding material. Along the principal symmetry direction *Γ- M,* 3200 m/s, sound velocities are found in Graphene. Graphene is very important from device point of view. In general flow of electrons is impeded by the presence of phonons. The dispersion of phonons is helpful in understanding the heat evolution and transmission in 2D materials. The phonon dispersion relations for Graphene has been plotted and utilized to study the phonon group velocities in these structures. The affect of phonon confinement on the two structures is different. Group velocity is suppressed in one case and enhanced in the other. Figure 2 show that the variation of ω with q is anomalous which has also been shown in the same figure (curved lines). There is considerable decrease in group velocity from its bulk value. The reduced group velocity will result in reduced thermal conductivity. This result has also been corroborated by Bo Peng *et al*. [9, 10].

5. Conclusion and Discussions

The present work is a systematic theoretical investigation of the elastic properties of Graphene. Based on the discussion above, it is important to note that the notion of using a simple interaction potential technique to calculate elastic coefficients for hexagonally organized 2D monolayer Graphene remains valid. The elasticity of materials concerns the cohesion of solids and the mechanical properties, such as phonon group velocities [10, 14]. In this regard, elastic constants are important parameters for construction of inter-atomic potentials and the mechanical stability of crystal. It indicates that Graphene is stable corresponding to shear. We have also calculated the values longitudinal and transverse sound velocities of monolayer Graphene. The calculated values of sound velocities would be compared with the available experimental data which shows a fairly good agreement [5, 9, 10]. Group velocity for some branches has been increased not only from there free standing value, but also from their bulk value. We derived the solution for the Γ and M points and numerically investigated the buckling effect on the material for phonon properties. We mainly fitted our model to account for the phonon group velocities [14].

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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] 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).

[6] 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).

[7] Novel Lattice Thermal Transport in Graphene Bo Peng, Hao Zhang, Hezhu Shao, Yuchen Xu, Xiangchao Zhang and Heyuan Zhu, Scientific Reports, August (2015).

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

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

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

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

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

[13] Kamlesh Kumar, M. Imran Aziz, Nafis Ahmad, IJSRST, 9 (2), 323-326, (2022).

[14] Kamlesh Kumar, Mohammad Imran Aziz, Khan Ahmad Anas, American journal of nanosciences, 13-18, (2022).

[15] Lele Tao, Chuanghua Yang, Liyuan Wu, Lihong Han, Yuxin Song, Shumin Wang, and Pengfei Lu, Modern Physics Letters B Vol. 30, No. 12, 1650146 (2016).

[16] Modarersi. M, Kakoee. A, Mogulkoc. Y, Comput. Mater. Sci., 101:164-167 (2015).