Graphene and Some of its Structural Analogues: 
Full-potential Density Functional Theory 
Calculations

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Abstract

Using full-potential density functional calculations we have investigated the structural and electronic properties of graphene and some of its structural analogues, viz., mono-layer (ML) of SiC, GeC, BN, AlN, GaN, ZnO, ZnS and ZnSe. While our calculations corroborate some of the reported results based on different methods, our results on ZnSe, the two dimensional bulk modulus of ML-GeC, ML-AlN, ML-GaN, ML-ZnO and ML-ZnS and the effective masses of the charge carriers in these binary mono-layers are something new. With the current progress in synthesis techniques, some of these new materials may be synthesized in near future for applications in nano-devices.

Keywords: Graphene, Graphene-like materials, 2D crystals, Electronic structure, Firstprinciples calculations

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1 Introduction

Graphene is a crystal of carbon (C) atoms tightly bound in a two dimensional (2D) hexagonal lattice. It is a monolayer of carbon atoms (ML-C), i.e., one atom thick. The exotic properties of this 2D material were revealed only in 2004-2005 by a series of papers coming from the Manchester [1–3] and Columbia [4] groups. The unambiguous synthesis (by mechanical exfoliation of graphite), identification (by transmission electron microscopy (TEM)) and experimental determination of some of the exotic properties of graphene were reported first in 2004, by the Manchester group led by Novoselov and Geim [1]. In 2010, Konstantin S. Novoselov and Andre Geim were awarded the Nobel Prize in Physics for the “groundbreaking experiments regarding the two-dimensional material graphene”. However, graphene research has a history which dates back to the 1859 work of Brodie [5–8]. The term graphene was introduced by Boehm and his colleagues in 1986 [9]. Graphene = “graph” + “ene” and the term “graph” is derived from the word “graphite” and the suffix “ene” refers to polycyclic aromatic hydrocarbons. Now graphene is considered as the basic building block of graphitic materials (i.e., graphite = stacked graphene, fullerenes = wrapped graphene, nanotube = rolled graphene, graphene nanoribbon = nano-scale finite area sized rectangular graphene).

The existence of free-standing 2D crystals were believed impossible for several years, because they would ultimately turn into a three-dimensional (3D) objects as predicted by Peierls [10], Landau [11] and Mermin [12]. The theoretical reason for this is that at finite temperatures, the displacements due to thermal fluctuations could be of the same magnitude as the inter-atomic distances, which make the crystal unstable. Further, experimentally one generally finds that thin films cannot be synthesized below a certain thickness, due to islands formations or even decomposition. Hence, the synthesis of graphene [1] was surprising which put a question mark on the predictions of Peierls, Landau and Mermin. However, this issue was (at least partially) solved when it was shown that freestanding graphene sheets display spontaneous ripples owing to thermal fluctuation [13], and therefore real graphene is not perfectly flat. It is important to note that such instabilities are the result of thermal fluctuations which disappear at temperature T = 0° K. This aspect will be used later in our discussions on the study of the stability of graphene and some of its structural analogues reported here on the basis of their ground state (i.e., T = 0° K) total energies.

Being a one-atom-thick planar crystal of C atoms, graphene is the thinnest nanomaterial ever known. It has exotic mechanical, thermal, electronic, optical and chemical properties, such as the high carrier mobility, a weak dependence of mobility on carrier concentration and temperature, unusual quantum hall effect, hardness exceeding 100 times that of the strongest steel of same thickness and yet flexible (graphene can sustain elastic tensile strain more than 20% without breaking, and is brittle at certain strain limit), high
thermal conductivity comparable to that of diamond and 10 times greater than that of copper, negative coefficient of thermal expansion over a wide range of temperature. Because of these properties graphene has potentials for many novel applications \[6,7,14,20\]. The rapid advancements of nanotechnology and the computing power have enabled the researchers in the field to explore the unusual properties of graphene from many perspectives of application and fundamental science. The study of graphene is possibly the largest and fastest growing field of research in material science.

The impressive growth in the research on graphene has inspired the study of other graphene-like 2D materials \[20,21\]. For instance, a number of 2D/quasi-2D nanocrystals (not based on carbon) have been synthesized or predicted theoretically in recent years. Representative samples of other 2D nanocrystals which have been synthesized include BN, MoS\(_2\), MoSe\(_2\), Bi\(_2\)Te\(_3\) \[20,21\], Si \[22\], ZnO \[23\]. Recently, the density functional theory (DFT) calculations of Freeman group \[24\] have shown that when the layer number of (0001)-oriented wurtzite (WZ) materials (e.g., AlN, BeO, GaN, SiC, ZnO and ZnS) is small, the WZ structures transform into a new form of stable hexagonal BN-like structure. This prediction has recently been confirmed in respect of ZnO \[23\], whose stability is attributed to the strong inplane sp\(^2\) hybridized bonds between Zn and O atoms. Graphene-like 2D/quasi-2D honeycomb structures of group-IV and III–V binary compounds have also been studied \[25,26\] by using pseudo-potential DFT calculations. Here, we report our calculations on the structural and electronic properties of graphene and some other graphene-like monolayer (ML) structures of the binary compounds, viz., SiC, GeC, BN, AlN, GaN, ZnO, ZnS, ZnSe using the DFT.

## 2 Computational Methods

We use the DFT based full-potential (linearized) augmented plane wave plus local orbital (FP-(L)APW+lo) method \[27-29\] as implemented in the elk-code (http:// elk.sourceforge.net/) and the Perdew-Zunger \[30\] variant of local density approximation (LDA) for our calculations. The accuracy of this method and code has been successfully tested in our previous studies \[31-37\]. For plane wave expansion in the interstitial region, we have used \(8 \leq |\mathbf{G} + \mathbf{k}|_{\text{max}} \times R_{\text{mt}} \leq 9\), where \(R_{\text{mt}}\) is the smallest muffin-tin radius, for deciding the plane wave cut-off. The Monkhorst-Pack \[38\] \(k\)-point grid size of \(20 \times 20 \times 1\) was used for structural and of \(30 \times 30 \times 1\) for band structure and total density of states (TDOS) calculations. The total energy was converged within 2 \(\mu\text{eV/atom}\). The 2D-hexagonal structure was simulated by a 3D-hexagonal super cell with a large value of \(c\)-parameter (\(= |\mathbf{c}| = 40\) a.u.) as shown in Figure 1. For structure optimization, we have considered two different structures, viz., (i) Planar structure (PL) and (ii) Buckled structure (BL) as shown in Figure 1 for a monolayer of BN (ML-BN), which is the prototype of all the
Figure 1: Two possible structures of ML-BN: Planar (PL) and Buckled (BL) in ball-and-stick model. Sub-figures (a) and (b) show the top-down views of ML-BN in PL and BL structure respectively. In the buckled ML-BN, B atoms (large balls, red) and N atoms (small balls, green) are in two different parallel planes (sub-figure (d)), buckling parameter $\Delta$ is the perpendicular distance between those parallel planes and $\Delta = 0$ Å for a flat ML-BN (sub-figure (c)). Sub-figures (e) and (f) respectively depict the 3D super cell of hexagonal BN in PL and BL structure with a large value of $c$-parameter (the length along the vertical axis).

3 Results and Discussions

We have optimized the 2D hexagonal structures of graphene (ML-C) and the monolayers of SiC (ML-SiC), GeC (ML-GeC), BN (ML-BN), AlN (ML-AlN), GaN (ML-GaN), ZnS (ML-ZnS) using the principle of minimum energy for the stable structure as per the following procedure. Initially we assumed the planar structures for all the materials considered here. With this assumption, we calculated the ground state in-plane lattice parameter ($a_0$) of each of these structures as listed in Table-1 along with the available reported values by other authors. Then we investigated the possibility of buckling in these structures at their assumed planar ground states (characterized by their respective $a_0$ values in planar states) by introducing the concept of bucking (Figure 1) and the
principle of minimum energy for the most stable structure. Our calculated variation of total energy (E) with buckling parameter (Δ) at fixed value of a₀ was then plotted to look for the value of Δ which corresponds to the minimum energy.

In Figures 2-4, we present our calculated results selecting one example from each group of materials considered here: graphene (ML-C) for Group-IV material, ML-BN for Group-III-V material and MLZnS for Group-II-VI material. As seen in the Figures 2-4, these structures have minimum energy at Δ = 0.00 Å, which means that these materials adopt 2D planar structures in the ground state (T = 0°K) unlike the case with silicene (graphene analogue of Si) [22, 31] that adopts a buckled structure in its ground state. It is to be noted that these results do not conflict with the theory of stability of 2D crystals [10–12]. Our calculated optimized structural parameters of the materials are listed in Table 1 along with available reported results based on other methods. The stability tests ML-ZnO and ML-ZnSe are not yet complete.

Considering the facts that LDA usually underestimates and GGA [39] usually over-estimates the lattice constant, the calculated value of a₀ slightly depends on the c-parameter used for super cells in DFT based calculations as we have seen before [31] for graphene (0.12% lower value of a for c → ∞) and silicene (0.075% lower value of a for c → ∞), and the different methods of study used by different authors, our results in Table 1 are acceptable.

Using the definition of the 2D bulk modulus of planar a graphene-like 2D material as

\[ B_{2D} = A \frac{\partial^2 E}{\partial A^2} \bigg|_{A_{min}} \]

(where A is the area of the periodic cell of the 2D lattice and \( A_{min} \) is the area with minimum energy), we have calculated the bulk modulus of each
Table 1: Calculated LDA values of ground state in-plane lattice constant \( a_0 (=|a| = |b|) \), buckling parameter \( \Delta \) of monolayer graphene (MLC) and some structurally similar binary compounds compared with available calculated data. PAW stands for the projector augmented wave.

| Material (2D) | \( a_0 \) (Å) | \( \Delta \) (Å) | Remark/Reference |
|---------------|----------------|-----------------|-----------------|
| ML-C          | 2.445          | 0.0             | Our Work/ [31, 33] |
|               | 2.46           | 0.0             | PAW-potential/ [25] |
|               | 2.4431         | 0.0             | Pseudo-potential/ [26] |
| ML-SiC        | 3.066          | 0.0             | Our Work/ [37] |
|               | 3.07           | 0.0             | PAW-potential/ [25] |
|               | 3.0531         | 0.0             | Pseudo-potential/ [26] |
| ML-GeC        | 3.195          | 0.0             | Our Work/ [37] |
|               | 3.22           | 0.0             | PAW-potential/ [25] |
| ML-BN         | 2.488          | 0.0             | Our Work/ [33, 34] |
|               | 2.51           | 0.0             | PAW-potential/ [25] |
|               | 2.4870         | 0.0             | Pseudo-potential/ [26] |
| ML-AlN        | 3.09           | 0.0             | Our Work/ [34] |
|               | 3.09           | 0.0             | PAW-potential/ [25] |
| ML-GaN        | 3.156          | 0.0             | Our Work/ [37] |
|               | 3.20           | 0.0             | PAW-potential/ [25] |
| ML-ZnO        | 3.20           | 0.0 (used)      | Our Work/ [35] |
|               | 3.283          | 0.0             | PAW-potential/ [46] |
| ML-ZnS        | 3.7995         | 0.0             | Our Work/ [36] |
|               | 3.890          | 0.0             | PAW-potential with GGA [39] / [47] |
| ML-ZnSe       | 3.996          | 0.0 (used)      | Our Work/ [37] |
Figure 3: Buckling probe of monolayer BN (ML-BN).

Table 2: Calculated 2D bulk modulus ($B_{2D}$) value of monolayer graphene and some other mono-layers of binary compounds in graphene-like structure compared with available calculated data using other methods. Our cited values of $B_{2D}$ from Wang [26] were obtained from Wang’s calculated values of 2D elastic constants $\gamma_{11}$ and $\gamma_{12}$ and another definition of $B_{2D} = (\gamma_{11} + \gamma_{12})/2$ [49].

| Material (2D) | $B_{2D}$ (N/m) | Remark/Reference               |
|--------------|----------------|--------------------------------|
| ML-C         | 223.85         | This Work                      |
|              | 214.41         | Pseudo-potential/ [26]         |
|              | 220.00         | Pseudo-potential/ [48]         |
| ML-SiC       | 125.66         | This Work                      |
|              | 121.945        | Pseudo-potential/ [26]         |
| ML-GeC       | 113.39         | This Work                      |
| ML-BN        | 188.03         | This Work                      |
|              | 181.91         | Pseudo-potential/ [26]         |
|              | 212.0          | Born’s Perturbation Method/ [49]|
| ML-AlN       | 113.44         | This Work                      |
| ML-GaN       | 109.45         | This Work                      |
| ML-ZnO       | 94.78          | This Work                      |
| ML-ZnS       | 53.94          | This Work                      |
| ML-ZnSe      | 48.57          | This Work                      |
of the materials considered here. These calculated values of $B_{2D}$ are listed in Table 2 along with the available calculated data based on other methods. As seen in Table 2, the 2D bulk modulus of graphene has the highest value and that of ML-ZnSe has the lowest value among the materials considered here, implying the fact that graphene has stronger in-plane bonds than the others and ML-ZnSe has the weakest bond among these materials. ML-GeC is seen to have same strength as that of ML-AlN. These data may be useful in selecting the 2D materials having desired level of strength in nano-mechanical applications in specific situations.

The LDA band structures of graphene (ML-C) and some other mono-layers of SiC, GeC, BN, AlN, GaN, ZnO, ZnS and ZnSe in graphene-like planar structure are depicted in Figure 5 and in Table 3, we have listed our calculated LDA values of the band gaps of these materials along with the reported values. As seen in the explicit case of ML-BN in Table 3, although LDA under-estimates the band gap (in our case the calculated value is about 23% less than the experimental value of 5.971 eV) it correctly predicts the nature of the gap. However, the use of a more advanced approximation, such as the LDA + GW$_0$ used in [25], improves the band gap problem (in the case of ML-BN although it overestimates band gap by 15% in this case), but the authors of [25] have presented their result in terms of an indirect band gap for ML-BN as opposed to the experimental observation of direct band gap in ref. [40]. In all other cases, the LDA nature of band gap is the same as that of the LDA + GW$_0$ band gap. The important point is that the actual band gap is always more than the LDA value.

Figure 4: Buckling probe of monolayer ZnS (ML-ZnS).
Table 3: Calculated LDA band gaps compared and listed with reported values.

| Material (2D) | \( E_g \) (eV) | Remark/Reference |
|---------------|----------------|------------------|
| ML-C          | 0 \((K \rightarrow K)\) | Our Work/[31,33] |
|               | 0 \((K \rightarrow K)\) | PAW-potential/[25] |
|               | 0                      | Pseudo-potential/[26] |
| ML-SiC        | 2.547 \((K \rightarrow M)\) | Our Work/[37] |
|               | 2.52 \((K \rightarrow M)\) | PAW-potential/[25] |
|               | 4.19 \((K \rightarrow M)\) | PAW-potential (LDA + GW\(_0\))/ [25] |
|               | 2.39                      | |
| ML-GeC        | 2.108 \((K \rightarrow K)\) | Our Work/[37] |
|               | 2.09 \((K \rightarrow K)\) | PAW-potential/[25] |
|               | 3.83 \((K \rightarrow K)\) | |
| ML-BN         | 4.606 \((K \rightarrow K)\) | Our Work/[33,34] |
|               | 4.61 \((K \rightarrow K)\) | PAW-potential/[25] |
|               | 6.86 \((K \rightarrow \Gamma)\) | PAW-potential (LDA + GW\(_0\))/ [25] |
|               | 4.35                      | Pseudo-potential/[26] |
|               | 5.971 (direct)            | Experiment/[40] |
| ML-AlN        | 3.037 \((K \rightarrow \Gamma)\) | Our Work/[34] |
|               | 3.08 \((K \rightarrow \Gamma)\) | PAW-potential/[25] |
|               | 5.57 \((K \rightarrow \Gamma)\) | PAW-potential (LDA + GW\(_0\))/ [25] |
| ML-GaN        | 2.462 \((K \rightarrow \Gamma)\) | Our Work/[37] |
|               | 2.27 \((K \rightarrow \Gamma)\) | PAW-potential/[25] |
| ML-ZnO        | 1.680 \((\Gamma \rightarrow \Gamma)\) | Our Work/[35] |
|               | 1.68 \((\Gamma \rightarrow \Gamma)\) | PAW-potential/[46] |
| ML-ZnS        | 2.622 \((\Gamma \rightarrow \Gamma)\) | Our Work/[36] |
|               | 2.07 \((\Gamma \rightarrow \Gamma)\) | PAW-potential with GGA/[39,47] |
| ML-ZnSe       | 1.866 \((\Gamma \rightarrow \Gamma)\) | Our Work/[37] |
Table 4: Calculated values of effective masses of the charge carriers in ML-C, ML-Si, ML-Ge, ML-BN, ML-AlN, ML-GaN, ZnO, ZnS, ZnSe. $m_0$ is the rest mass of electron.

| Material (2D) | Effective mass ($m_0$) | Remark/Reference |
|---------------|-------------------------|------------------|
| ML-C          | $m_e(K) = 0$            | This Work        |
|               | $m_h(K) = 0$            | This Work        |
| ML-SiC        | $m_e(M) = 0.411$        | This Work        |
|               | $m_h(K) = -0.488$       | This Work        |
| ML-GeC        | $m_e(K) = 0.509$        | This Work        |
|               | $m_h(K) = -0.400$       | This Work        |
| ML-BN         | $m_e(K) = 0.920$        | This Work        |
|               | $m_h(K) = -0.617$       | This Work        |
| ML-AlN        | $m_e(\Gamma) = 0.523$  | This Work        |
|               | $m_h(K) = -1.470$       | This Work        |
| ML-GaN        | $m_e(\Gamma) = 0.266$  | This Work        |
|               | $m_h(K) = -1.157$       | This Work        |
| ML-ZnO        | $m_e(\Gamma) = 0.253$  | This Work        |
|               | $m_{hh}(\Gamma) = -0.793$ | This Work    |
| ML-ZnS        | $m_e(\Gamma) = 0.173$  | This Work        |
|               | $m_{hh}(\Gamma) = -0.665$ | This Work    |
| ML-ZnSe       | $m_e(\Gamma) = 0.107$  | This Work        |
|               | $m_{hh}(\Gamma) = -0.652$ | This Work    |
In Table 4, we present our calculated values of the effective masses of the charge carriers in ML-C, ML-Si, ML-Ge, ML-BN, ML-AlN, ML-GaN, ZnO, ZnS, ZnSe, determined at the band edges at the special points as appropriate for the material under study. From the linear energy dispersion close to the $K$ point of the hexagonal Brillouin Zone (BZ) as shown in Figure 6, mass-less carriers in graphene were inferred. As seen in Figure 6, near the $K$ point of the BZ, the energy band dispersion is linear in $k$:

$$E_{\pm} = \pm v_F \hbar k$$

where $v_F$ is the magnitude of Fermi velocity of the charge carriers in graphene and $(\hbar k)$ is the magnitude of the momentum. Thus, charge carriers in graphene behave like mass-less relativistic particles. From the slope of the linear bands one obtains the value of $v_F$, which in our calculation corresponds to $v_F = 0.8327 \times 10^6$ m/s. This value of $v_F$ is close to the
experimentally measured value of $v_F = 0.79 \times 10^6 \text{ m/s}$ in graphene monolayer deposited on graphite substrate \cite{41} and the reported calculated LAPW value of $0.833 \times 10^6 \text{ m/s}$ \cite{42} and about 20\% less than that measured in coupled multi-layers \cite{43,44} and the tight-binding value: $v_F = 1 \times 10^6 \text{ m/s}$ \cite{15}. The smallness in the value of $v_F$ in ref. \cite{41} was attributed to the electron-phonon interactions due to strong coupling with the graphite substrate. However, the closeness of our calculated value of $v_F$ for a freestanding graphene monolayer with the results of ref. \cite{41} suggests a very weak coupling of graphene to the graphite substrate used in ref. \cite{41}. Surprisingly, our calculated value of $v_F$ is close to the measured value of $v_F = 0.81 \times 10^6 \text{ m/s}$ \cite{45} in metallic single-walled carbon nanotube.

4 Conclusions

Using full potential DFT calculations we have investigated the structural and electronic properties of graphene and some other graphene-like materials. While our results corroborate the previous theoretical studies based on different methods, our calculations on ML-ZnSe, the two-dimensional bulk modulus of ML-GeC, ML-AlN, ML-GaN, ML-ZnO, ML-ZnS, and the effective masses of the binary monolayer compounds considered here are our new results. We hope, with the advancement of fabrication techniques, the hypothetical graphenelike materials discussed here will be synthesized in the near future for potential applications in a variety of novel nano-devices.


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