Ab-Initio Investigations on Structural, Electronic and Optical Behaviours of Graphene/h-BN Based Layered Systems

Muhammad Talha[#1,3], Muhammad Rafique[#1,2,*], Irfan Ahmed[#1] and Yong Shuai[#2]

[#(1)]*Mehran University of Engineering and Technology, SZAB, Campus, Pakistan*

[#(2)]*School of Energy Science and Engineering, Harbin Institute of Technology,92 West Dazhi Street, Harbin 150001, PR China*

[#(3)]*Benazir Bhutto Shaheed University of Technology and Skill Development, Khairpur Mirs', Pakistan*

Abstract

This paper deals with the structural, electronic and optical characteristics of graphene and h-BN materials based few layered systems adopting first-principles DFT method. Graphene and h-BN 2D materials were stacked in layers using homo and hetero-structures configurations and aforementioned properties of few layered systems were observed in detail. In terms electronic behaviours, of pure bilayer graphene and h-BN systems display similar trends as that of their single layer counter-part but with quantitative increase in its physical properties. When graphene and h-BN layers are stacked together, this produces a conducting material behaviour having 0.5 eV band gap. After inclusion of single h-BN layer in between two graphene layers, the resultant is a layered graphene-like material having secondary Dirac point formation at the high symmetric point. When graphene is stacked between two h-BN layers, the resulting structure displays semimetal behaviour, thus converting wide band insulating h-BN layers to semi metallic state. Through optical properties (i.e., absorption and reflectivity) it was found that, single graphene and single h-BN stacking produces an absorptive material for visible range of spectrum. Similarly, graphene-h-BN -graphene stacked shows improved absorption in visible energy range. The static reflectivity of graphene-h-BN -graphene and h-BN-graphene-h-BN gains 0.7 intensity peak values as compared to pure bilayer graphene and bilayer h-BN systems. Outcomes of this study suggest that, combining graphene and h-BN 2D materials in stacked formation can produce functional opto-electronic materials for real engineering applications and these results can further be experimentally extrapolated.

Keywords — *Bilayer graphene; bilayer h-BN; Band gap; Absorption; Reflectivity; DFT*

I. INTRODUCTION

After the extraction of monolayer graphene by Novoselov and Geim in 2004 [1], this material brought with itself exhilarating electronic parameters behaviours, graphene electrons exhibit massless Dirac-fermions dispersion behaviour at the E_F (Fermi energy) level [2, 3]. Monatomic graphene produces unique characteristics [3-6] for instance, Quantum-Hall effect [5, 7], Kohn-Sham irregularity [8, 9] and the optical conductance in infrared (IR) region [10-13]. Additionally, the massless electron behaviour and 2D lattice structure of graphene makes it optimal choice for high frequency electronic circuit devices, which can be designed in atomic-scale range without miniaturization of 3D materials [14-16]. Even with such distinctive characteristics, graphene suffers zero band-gap dilemma, hence its conductance cannot be controlled through external voltages; that is a crucial part of all the functional electrical and electronic devices [17, 18].

Very recently, some studies have been performed on few layered graphene (FLG) systems, subjected to band gap engineering through symmetry variation and inter-atomic structure modification [19, 20]. Very commonly used methods for functionalization of layered systems is through electrical doping [21, 22] and chemical doping [23, 24]. Some experimental are also being carried out on intercalated FLG systems [25-27] for band-gap modification so that a functional layered system can be synthesized for nano-electronic devices. Recently, H. Jinsen et al. [28] investigated transition metal atoms (TMA) intercalated BLG systems through FPS-DFT technique; authors suggested that, the TMA intercalation in BLG converts it to a stable 2D magnetic substrate from a nonmagnetic material. Though, foreign atoms/clusters intercalation in

layered systems can produce functional materials, but it becomes near impossible to experimentally investigate and synthesize intercalated layered systems due to the interlayer distance being in nm range [25, 29, 30]. Alternatively, the adsorption, substitution of foreign atoms on the surface or in layers is a practicable move towards experimental realization of such systems [25, 31]. Further, stacking of hetero-structures can also generate novel materials with desired electronic properties. Thus, our work is focused on stacking of h-BN and graphene layers with varying layer numbers, so that a significant band gap can be induced in the electronic structure graphene layers. Due to insulting behaviour of h-BN system, it was selected as stacking layer, so that it can add some of its behaviours in the electronic structure of graphene layers. In addition to electronic properties, we also investigate the optical behaviours (i.e., absorption and reflectivity) of layered systems. Since, through stacking of various layers, electronic properties can be modified, which in turn produces variations in inter/intra band transitions, thus resulting modified optical behaviours of layered systems. Noteworthy literature is already available on layered graphene-h-BN systems, while varying layers numbers configurations has been slightly studied and their effects on the electronic and optical characteristics are thoroughly investigated.

Our work organization is as follows: computational details and geometry of layered systems is explained in Sec II; electronic, optical parameters of pristine graphene, h-BN and hetero-structures stacked complexes are discussed and analysed in Sec III; lastly Sec IV, illustrates a general conclusion and summary of this work.

II. GEOMETRY AND COMPUTATIONAL DETAILS

Adopting first-principles DFT calculations within Generalized Gradient Approximation (GGA) [32, 33] using VASP software [34, 35], we investigated the electronic and optical properties of stacked layers (i.e., graphene and h-BN). All the calculations are carried out on a 4 × 3 bilayer supercell arrangement [36, 37] with plane-wave basis adopting ultrasoft psuedopotentials [34, 38] with 500 eV cut-off-energy. A vacuum thickness of 15 Å is added along the Z-direction, in order to evade the spurious interaction between neighbouring layers. Various configurations such as graphene-graphene, h-BN-h-BN, graphene-h-BN, graphene-h-BN-graphene and h-BN-graphene-h-BN of layers were studied and the resulting electronic and optical parameters of said systems were studied in detail. A 17 × 17 × 1 k-point mesh is utilized for good convergence criteria. Relaxation was performed until, less than 0.03 eV/Å Hellmann-Feynman forces and 10-6 eV total change in energy parameters were achieved. Gaussian smearing is done for partial occupancies. Relaxed geometries of pure 4 × 3 graphene-h-BN, graphene-h-BN-graphene layered structures are presented in Figs. 1(a)-1(b), respectively.

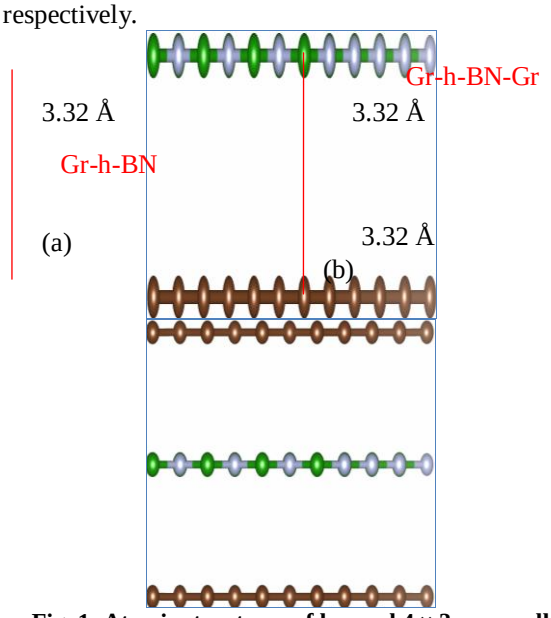

Fig. 1: Atomic structures of layered 4 × 3 supercell hetero-structures.

Thirty points are utilized through Gamma- M - K - Gamma path in the I.B. (irreducible Brillouin) zone for electronic structure calculations, in order to extract a band structure with fine grid. For eigenvalues smearing a 0.02 eV Gaussians of width was employed. Similarly, for optical parameters, Random Phase Approximations (RPA) technique within DFT [39] is employed. It is well known that, various optical properties can be extracted from dielectric constant, thus it's necessary to calculate dielectric constant first. Through empty states summation process, the imaginary dielectric constant can be determined as expressed below;

$$\varepsilon''_{\alpha\beta}(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \sum_{c,v,k} 2\omega_k \, \delta(\epsilon_{ck} - \epsilon_{vk} - \omega) \; u_{ck+e_\alpha q} | u_{vk} u_{ck+e_\beta q} | u_{vk} \quad (1)$$

Here, α and β are Cartesian vectors, e_α / e_β are primal vectors of single unit cell and the terms c/v represent conduction/valence bands, in that order. Corresponding energy of c/v bands is presented by $\epsilon_{ck} / \epsilon_{vk}$ parameters accordingly, cell periodic part at a given point k is denoted u_{ck} term.

For real dielectric constant, Kramers-Kronig transformation technique is employed as expressed below; here the term P describes Principal value. Detailed explanation of this technique is provided in Ref. [39].

$$\varepsilon'_{\alpha\beta}(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\varepsilon''_{\alpha\beta}(\omega')\omega'}{\omega'^2 - \omega^2 + i\eta} d\omega' \qquad (2)$$

After successful extraction of real and imaginary dielectric constant values, complete dielectric constant can be obtained by $\varepsilon = \varepsilon' + i$ together [39]. The optical absorbance 'α' and reflectivity 'R' can easily be calculated from the dielectric constant quantity [40, 41]. In terms of optical parameters, the focus of this work lies in low electron energy range i.e., in between 0-10 eV energy. Main idea of this work is to investigate and improve the absorption spectra of layered 2D systems in visible range. Furthermore, the static reflectance of all layered hetero-structures is investigated. Layered hetero-structures with enhanced optical parameters in visible range can be utilized for opto-electronic application comparative to hybrid single layered systems as well as doped/intercalated few layered systems.

III. RESULTS AND DISCUSSIONS

Outcomes of this study along with appropriate analysis and discussion follow as under:

A. Structure diagrams of layered heterostructures

Layered graphene/h-BN systems with varying layer numbers were investigated in this paper. Structure and electronic properties of hetero-structures are calculated and analysed in this section. Geometry relaxation is performed for all these systems, in order to obtain the stable systems on which further calculations can be performed. To fully understand the change in the atomic structure and interlayer variation, no constraints were performed; rather they were relaxed during optimization process.

Typical relaxed geometries of layered systems are presented in Figs. 2(a)-(e), respectively. Optimized geometries of given systems illustrated in Figs. 2(a)-(e) indicate that, interlayer distance variation is dependent upon the type of layers being stacked. Van der Waals interaction also plays a significant part is bond length variation in between constituent C-C and B-N atoms, respectively. Interlayer distance variation observed was in range of 3.13-4.01 Å, correspondingly. Our results are in consensus with earlier reports [42-45].

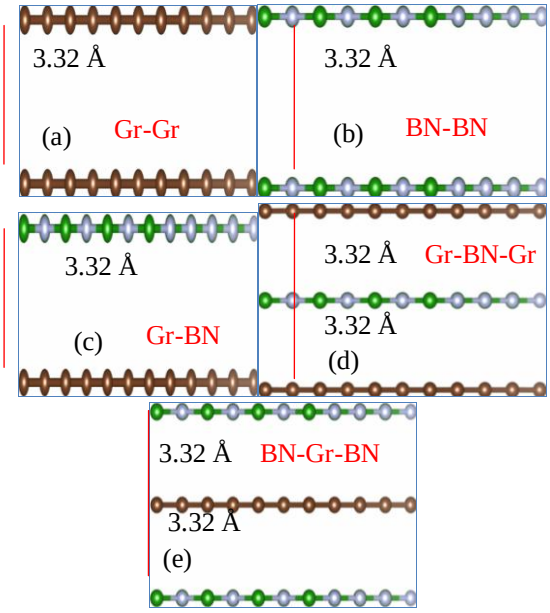

Fig. 2: Atomic structures of 4 × 3 supercell hetero-structures with interlayer distance given in Å, respectively.

B. Electronic structures of layered heterostructures

Band structures of pristine bilayer and h-BN systems are shown in Fig. 3(a) and (b), respectively. Specific electronic structure of bilayer graphene i.e., quadratic dispersion at the Dirac point and touching of valence and conduction bands at the E_F level is described clearly in Fig. 3(a) [46].

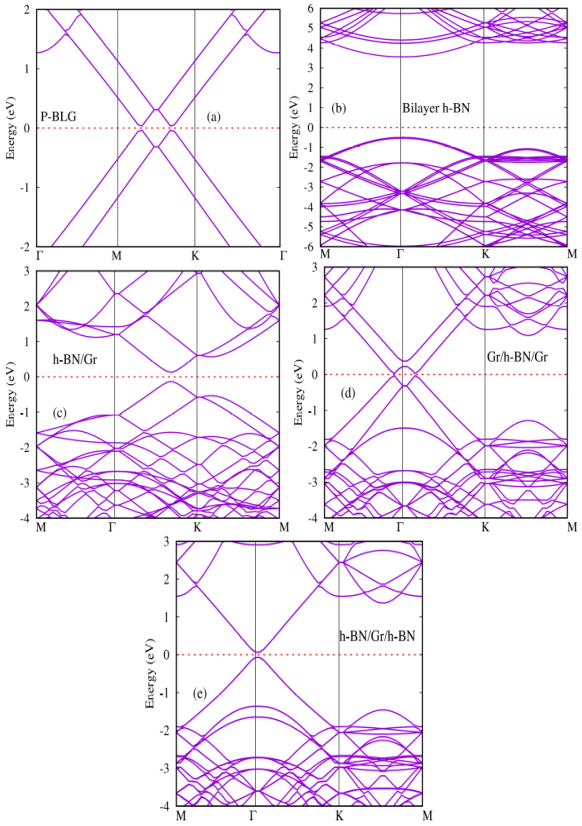

Fig. 3. Electronic band structures of 4 × 3 supercell hetero-structures, graphene is represented by (Gr).

Similarly, electronic structure of bilayer h-BN also shows insulating behaviour with 3.92 eV band gap as seen in Fig. 3(b) [47]. These results agree well with earlier reports, suggesting that our computational technique is accurate enough to proceed further. The electronic structures of layered h-BN/graphene, graphene/h-BN/graphene, h-BN/graphene/h-BN are shown in Figs. 3(c)-(e), respectively. As seen in Fig. 3(c), stacking of h-BN and graphene produces a conducting material with band gap of 0.4 eV. Stacking of graphene/h-BN/graphene produces a half metal layered system as some surface states appear at the E_F level and formation of binary Dirac point happens. Similarly, when graphene is stacked in between two h-BN layers, a semi-metal material is obtained with 0.3 eV band gap value as shown in Fig. 3(e), respectively. In general, it can be suggested that, stacking of h-BN and graphene layers produces an intermediate layered system which mimics the properties of both graphene and h-BN, some conducting and semimetal materials are obtained from stacked configurations. These results are consistent with earlier studies [31, 48-51].

C. Optical parameters of layered heterostructures

Lastly, we calculate the optical behaviours specifically (absorption coefficient and reflectivity) of various layered hetero-structures. As discussed, exciting electronic properties of graphene produce distinctive optical behaviours. Similarly, h-BN layer also carries unique optical behaviours individually. Stacking these two materials can produce a novel set of optical properties which arise from two distinct contributions, i.e., inter/intraband transitions [12, 52]. Pristine bilayer graphene, h-BN layers and stacked hetero-structures optical absorbance 'α' and reflectivity 'R' parameters are investigated and presented in Fig. 4(a) and (b), respectively. It seems that, first principal peak of pristine bilayer appears at 3.8 eV, energy and for pristine h-BN it appears at 7 eV, energy as shown in Fig. 4(a). For better comprehension of results, the absorption coefficient plot is drawn in between 0-10 eV energy range. After stacking of graphene and h-BN layers with varying concentration, first minimum peak associated to $\pi \rightarrow \pi^*$ transition shifts towards lower energy range as evident in Fig. 4(a). Furthermore, the absorbance starts from 0 eV energy range, whereas for both pure bilayer graphene and h-BN, have no absorbance in low energy range. It can be suggested that, stacking of graphene and h-BN can produce a unique material which can absorb in visible energy range as a red shift towards visible range of spectrum is obtained after stacking of graphene and h-BN layers.

The reflectivity 'R' parameter of all stacked systems is illustrated in Fig. 4(b). The static 'R' for pristine bilayer graphene is found to be 0.28 and for pure bilayer h-BN is 0.1 as evident in Fig. 4(b). However, it can be observed from Fig. 4(b) that, stacking of these layers causes a significant rise in the static 'R' parameter as visible in Fig. 4(b). Calculated static reflectivity peak intensity values are 0.7, 0.68 and 0.23 for h-BN/graphene, graphene/h-BN/graphene and h-BN/graphene/h-BN stacked structures as shown in Fig. 4(b), respectively. In conclusion, it can be predicted that, stacking of layers can result is improved static 'R' parameter. Acquired optical parameters of stacked systems agree well with previous studies [53-55].

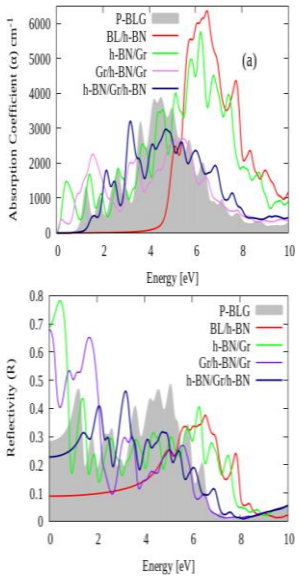

Fig. 4. Optical characteristics of 4 × 3 supercell hetero-structures, graphene is represented by (Gr).

IV. CONCLUSIONS

In summary, ab initio electronic structures and optical parameter investigations pristine bilayer graphene and h-BN systems along with stacked graphene/h-BN systems are investigated. Band gap engineering is done through stacking of graphene/h-BN layers with varying layer numbers. Obtained results are partially in consensus with earlier studies. It is found that, stacking of h-BN and graphene layers together can produce conducting/half metal/semimetal materials depending upon the stacked configuration of layers. A finite band gap in between 0.3 eV and 0.5 eV is achieved in the electronic structures of stacked systems. From the first-principles electronic calculations it can be summarized that, stacked hetero-structures systems can easily be converted to conducting/half metallic materials through controlled stacking of graphene and h-BN layers.

The optical absorbance 'α' and reflectivity 'R' are calculated for pristine bilayer graphene and h-BN, as well as for stacked hetero-structures in low electron energy range. Obtained results suggest that, graphene and h-BN stacking improves static reflectivity parameter of layered systems, while producing minimum variations in 'R' parameter in higher energy range. Similarly, new optical absorbance 'α' peaks is generated in 0-2 eV energy range after stacking of graphene/h-BN layers. It should be noted here that bilayer graphene and h-BN has no optical absorption in between 0-1 eV energy. However, after stacking minor peaks are generated along with absorption quantity being starting from 0 eV energy range. Results obtained during this work offer a viable approach for band gap engineering and optical properties manipulation in multilayer systems, also predicting the possibility of designing multilayer graphene and h-BN based optical materials functional for opto-electronic and solar energy applications.

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