Computational Investigations On Opto-Electronic Properties Of Carbon (C) Atom Doped Monolayer Aln Systems Using Ab-Initio Method

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Abstract
With the help of ab-initio computational technique, opto-electronic properties of carbon (C) atom substituted monolayer Aluminium Nitride (AlN) systems are invetigated. In this study, C atoms were placed in AlN layer with varying concentration and the effects of C atom-doping on optical and electronic properties were investigated in detail. It is well known that, AlN is a wide band material with 3.92 eV band gap. When C atoms are placed in AlN layer, the electronic behavior is modified, i.e. converts wide band AlN layer to half metal/semimetal/conducting material depending upon the number of C atoms present in AlN lattice. When two C atoms replaced Al atoms in AlN lattice, some impurity states appeared at the Fermi level, thereby making half metal material. When two C atoms replaced two N atoms in AlN layer, it displayed semimetal property having almost negligible band gap. Upon substituting 4 C atoms in AlN layer, a conducting AlN material was achieved having band gap of ~0.7 eV in its electronic structure. Similarly, when 6C atoms replaced a whole AlN ring, a semiconducting C-AlN hybrid material was obtained having 2.2 eV band gap in its electronic structure. Using random phase approximation (RPA) technique implemented with density functional theory (DFT), the optical absorbance and reflectance parameters were investigated for pure and C doped AlN systems. For pure AlN system, we have zero absorption quantity in between 0-8 eV energy and have almost negligible static reflectivity parameter. However, when various C atoms were placed in AlN lattice, the optical absorbance is improved in low lying energy range, suggesting a red shift towards visible region of spectrum. The static reflectivity parameter was also improved after C atom substitution and reflectivity is reduced in higher energy range. Opto-electronic properties of C atom-doped AlN systems gained in this system suggest that, C atom substitution in AlN layer is a viable technique to manipulate its physical trends, in order to make it functional for opto-electronic device applications which are distinctive to pristine AlN system

Keywords— Monolayer AlN; Carbon doping; Electronic structure; Optical properties.

I. INTRODUCTION

In the past decade, various two-dimensional (2D) hexagonal structures such as graphene [1-3], h-BN [4], MoS_2 [5], SiC [6] and ZnO [7] have been experimentally studied on a large scale, and their intrinsic and defect states have been extensively analysed in the research community. Among these 2D materials, Group III-nitrides show great potential for real engineering applications such as semiconductor lasers, LEDs, power electronics, optical sensors/detectors and visible light photocatalysis of water [8-11]. These transition metal nitrides with sufficient energy gap have received much attention due to their photonic and optoelectronic device applications [12-14]. From the transition metal-nitride family, a single layer of AlN [15] with a band gap of 3.92 eV appears to be a promising dilute magnetic semiconductor (DMS) materials. The AlN nanowires were synthesized by Wu et al. [16] using different fabrication and growth methods. Zhou et al. [17] studied the electronic parameters of AlN nanotubes and nanowires. In their work, the authors also pointed out that, AlN nanostructures may be potential candidates for ammonia sensor applications. Similarly, by Xie et al. [18] 1D nanoribbons of pure AlN were synthesized by a chloride-assisted vapor-solid route. Even with such a successful AlN nanostructure fabrication process, there is little literature available on the basic physical properties of AlN nanostructures.

Recently, h-GaN and h-AlN have gained further importance due to the realization of ultra-thin AlN and GaN in a honeycomb structure. Tsipas et al. [19] studied the epitaxial growth of ultra-thin hexagonal AlN on single crystal Ag (111) in 2013. Recently, few single-layer thick plane h-AlNs have been formed on the Si(111) surface by molecular

beam epitaxy and lattice constant 3.08Å was obtained [20]. In addition, 2D GaN has been synthesized by graphene encapsulation [21]. Theoretical and experimental studies have shown that single-layer h-GaN and h-AlN are indirect wide-bandgap semiconductors. They are easy to form two-layer and multi-layer, even h-GaN/h-AlN heterostructures, whereby the electronic and optical properties can be adjusted by the number of layers [22-24]. Other efficient ways to modify and hence to attain diverse physical properties have been the chemisorption/chemical doping of foreign atoms or molecules, substitution of host atoms by other atoms and creation of patterned vacancies or di vacancies in these 2D structures [25, 26]. Here, one expects that chemical doping or substitution of foreign atoms and creation of vacancies in low (dilute) concentration scan give rise to localized states in the fundamental band gap and resonance states in the band continua. Accordingly, the electronic structure of h-AlN and h-GaN are modified due to acceptor and donor or simply impurity states in the fundamental bandgap, the energies of which vary depending on the type foreign atom and type of the vacancy. The localized states are broadened and form impurity bands with increasing coupling among impurities at higher concentrations. Additionally, owing to the unpaired electrons local magnetic moments attribute magnetic properties. Earlier, it has been shown that band gap is reduced when extended line defects are introduced into the honeycomb structures of h-AlN and h-GaN monolayer [27]. Much recently, theoretical studies have been published about magnetism due to the adsorption of some non-metal atoms to h-GaN [26] the adsorption of O and Pt atoms and their clusters on h-AlN [27], Mg doping of h-AlN [28] and h-GaN and Ga or N single vacancy charged defects in h-GaN [29].

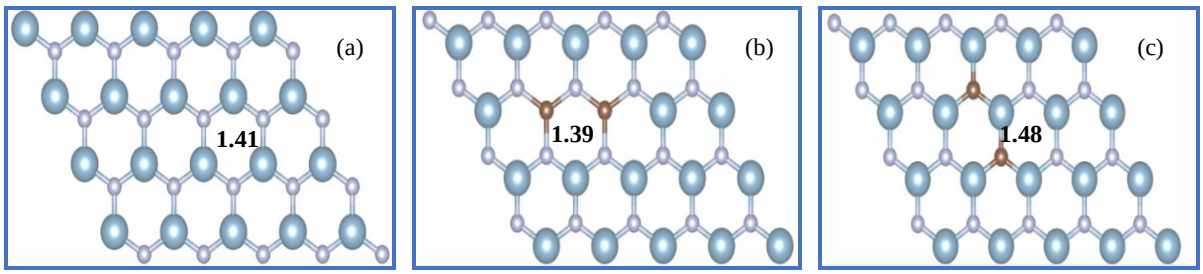
I. Computational details

First-principles density functional theory investigations were performed using VASP simulation package [30, 31] with PAW (projector augmented wave) scheme [32]. PBE (Perdew–Burke–Ernzerhof) function [33] with GGA (generalized-gradient approximation) technique was utilized for exchanges and correlations. Structure model consist of 4 × 3AlN supercell having 20 Å in Z-direction, on which 450eV cut-off energy was applied for expansion of its plane waves. Brillouin zone (BZ) was sampled using 7×7×1*Gamma*-centered k-mesh. C atom-doped AlN systems were optimized till the Hellmann–Feynman force and total energy parameters did not gain 0.02 eV/Å and 10^{-5} eV values, respectively. Band structure was calculated using 30 points along *Gamma- M - K - Gamma* path in the irreducible BZ, in order to gain fine quality electronic structures. For optical parameters, Random Phase Approximation (RPA) technique was adopted. Brief explanation on the extraction of optical parameters can be easily found in previous studies [34, 35].

II. Results and discussions

Firstly, we investigated pure AlN sheet and its optimized geometry is shown in Fig. 1 (a). The lattice constant was found to be 2.45 Å which is nearly same as the experimental value of 2.46 Å and the Al-N atoms bond length was found to be 1.418 Å which is in agreement with the previous work [36, 37]. We calculated the band structure of pure AlN and is shown in Fig. 2(a). Our calculated band structure of pure AlN is in good agreement with the previous studies in terms of gapless behavior and linear dispersion of energy at the Fermi level [38-40].

Later, we investigate the effect of C doping on the electronic and optical properties of AlN. We use C atom doping configuration in the form of ring doping with varying concentration of 6.25 % (2 C atoms in AlN layer) to 18.75 % (6Catoms doped AlN layer). When Al is doped with 6.25 % dopant concentration, N-C bond length is found to be 1.396 Å, Al-C bond length is 1.472 Å and Al-N bond length is 1.435Årespectively. However, when the concentration of dopant atoms is increased to 18.75 % the bond lengths are further reduced, N-C bond length is found to be 1.384 Å, Al-C bond length is 1.461 Å and Al-N bond length is 1.414Årespectively. Optimized geometries of various C atoms doped AlN layers are presented in Fig. 1(b)-(e), respectively.



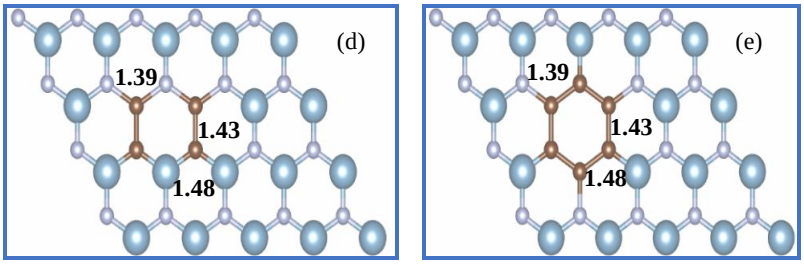


Fig 1: Optimized structure of (a) pure AlN (b) 6.25 %dopant concentration 2 C co-doped Al (c) 6.25 % dopant concentration 2 C co-doped N (d) 6.25 % dopant concentration dopant concentration 4C co-doped AlN and (e) 18.75 % dopant concentration dopant concentration 6C co-doped AlN. Gray, Green and light blue balls indicate Al, N and C atoms, respectively.

IV. BAND STRUCTURE AND DENSITY OF STATES

Band structure diagrams of pure and 25 % and 41.67 % C co-doped AlN are shown in Fig. 2(a)-(e), respectively. Band structure of pure AlN layer shown in Fig. (a) indicates that, it is a wide band semiconducting material having 3.92 eV band gap. Fermi energy (E_F) level is shown by dotted red color line in the electronic structures. Obtained electronic structure of pure AlN layer is in consensus with earlier studies [41-43]. Satisfactory result of electronic structure of AlN layer suggests that, our computational technique is reliable and it can be employed to calculate the electronic parameters of various C atom-doped monolayer AlN systems.

It can be observed from the electronic structures provided in Figs. 2(a)-(e), that the C atom substitution in AlN layer causes variation in energy gap, as well as changes the placement of Fermi level. However, for understanding purpose, the Fermi energy level is fixed at 0 eV energy. As shown in Fig. 2(b) that, when two C atoms replace two Al atoms in AlN lattice, the insulting AlN layer is converted to a half metal material since few surface states are available at the Fermi energy level. When two C atoms replace two N atoms, the wide band AlN system is converted to semimetal having almost negligible band gap as shown in Fig. 2(c). When 4C atoms are placed in AlN lattice, a conducting AlN layer is obtained having ~0.7 eV band gap as visible in Fig. 2(d). Lastly, when 6C atoms are embedded in AlN layer, a semiconducting AlN layer with 2.2 eV band gap is achieved as seen in Fig. 2(e). From the electronic structures shown in Fig. 2(a)-(e), it can be summarized that the C atoms greatly modify the electronic structure of AlN layer, in addition, the energy gap is sensitive to the concentration of C impurities as well. This technique offers a feasible approach to modify the electronic structure of AlN system through hetero-atom substitution.

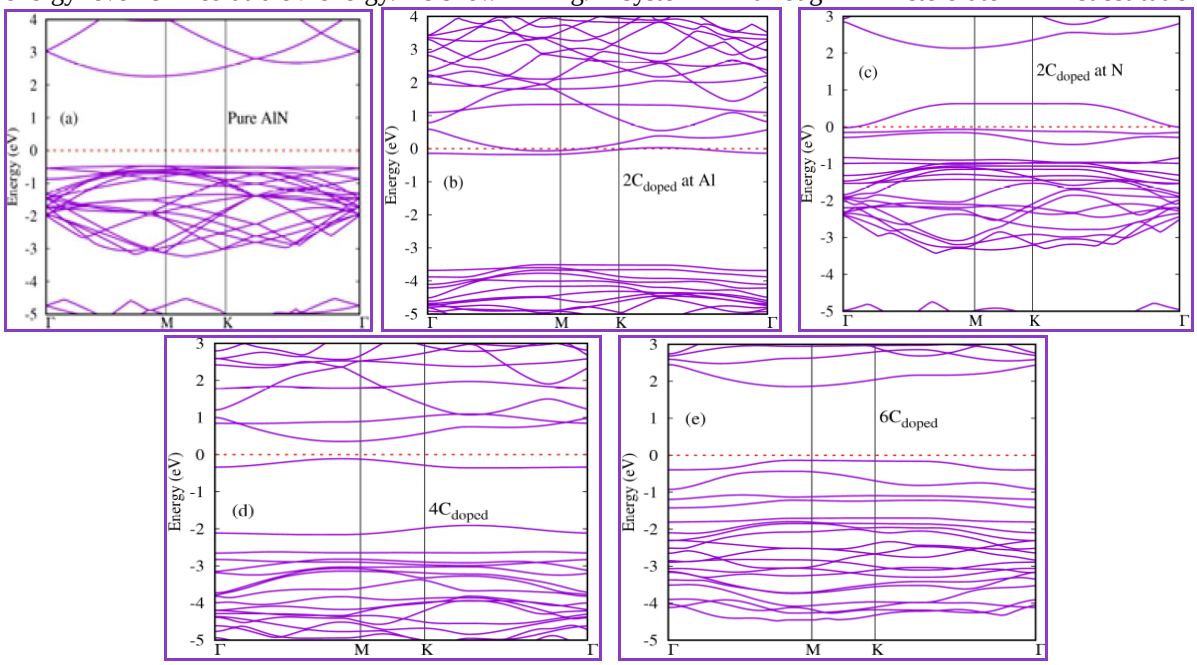


Fig 2: Illustration of band structures of (a) Pure AlN (b) 2C doped at Al (c) 2C doped atN (d) 4C doped AlN and (e) 6C doped AlN respectively.

IV. OPTICAL PROPERTIES

In order to calculate the optical properties, we used DFT within the Random Phase Approximation (RPA) [44] approach in which local fields effects are omitted. Only inter band transitions are included, so there can be some inaccuracy in dielectric function at low energies. Firstly, dielectric constant 'ε' was calculated. Since dielectric constant is the sum of real and imaginary part i.e. ε = ε' + i ε" together. The imaginary part is obtained by the summation of empty states and the real part of dielectric tensor was calculated using Kramers-Kronig transformation [44]. After getting dielectric tensors, we can easily calculate absorption coefficient 'α' and reflectivity 'R' [35, 45].

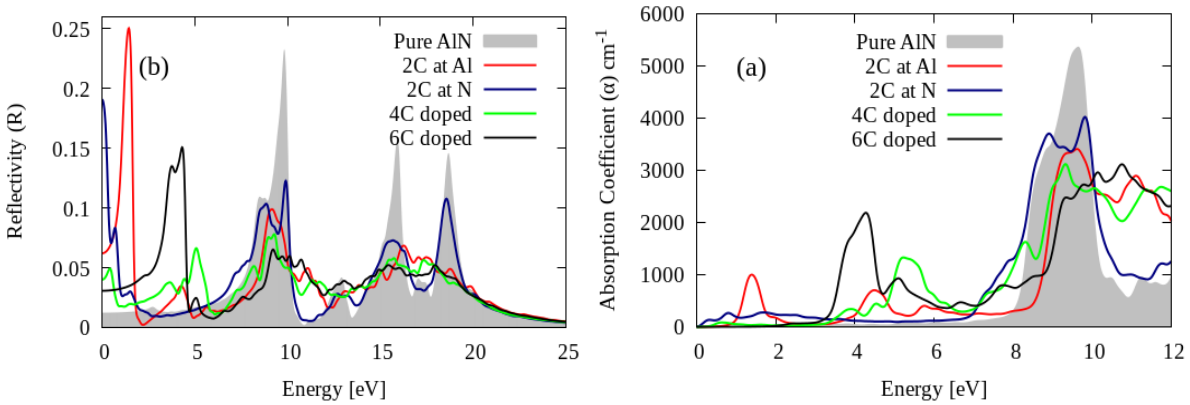


Fig 3: Illustration of (a) Absorption coefficient and (b) Reflectivity of pure and variants C atom doped AlN system

The grey color shows absorption coefficient and reflectivity plots for pure, AlN and red indicate 2C doped Al, blue indicate 2C doped at N, green indicate 4C doped and black indicate 6C doped rings-doped AlN which are shown in Fig. 3(a) and 4(b), respectively. In absorption plot of pure AlN, there is a peak present at the energy levels of 9.5eV energy as shown in Fig. 4(a). However, after C ring doping the absorption coefficient peaks intensities are reduced. An interesting phenomenon occurs after C doping, that is the absorption coefficient shifts to visible region. In case of 2C doping at Al with a peak intensity of 1000 cm^{-1} at 1.5 eV, 2Cat N rings doping produces no any significant variation in absorption, after 4C doped AlN peak intensity appear at 5.5 eV with 1200 cm^{-1} peak intensity respectively as shown in Fig. 3(a). Significantly it can be observed that 6C substitution causes a larger peak value of 2200 cm^{-1} at 4 eV. It can be summarized that C atom substitution in AlN material can produced absorption in visible energy range. Reflectivity plots shown in Fig. 3(b) indicate that C co-doping causes overall reduction in the reflectivity of AlN in low energy region. Static reflectivity peak values for pure, 2C at Al, 2C at N, 4C and 6C doped AlN system are found to be 0.02, 0.07, 1.8, 0.03 and 0.04 respectively. It can be summarized that C doping cause overall cause overall reduction inn reflectivity at higher energy level while the minor changes to the static reflectivity parameters [35, 46].

IV. FORMATION ENERGIES

In order verify the stable nature of C atom-doped monolayer AlN systems, the formation energies for given systems were calculated using following expression [47],

$$E_{f(AlN-C)} = E_{(AlN-C)} - E_{AlN} + l\mu_{Al} + m\mu_N - n\mu_C$$

here, the terms E_{AlN} and $E_{(AlN-C)}$ define the energies of pure and C substituted AlN systems, in that order. The chemical potentials of carbon μ_c, aluminium μ_{Al} and nitrogen μ_N were obtained from pristine graphene and pristine AlN systems [39, 48]. The coefficients l, m represent number of Al, N atoms being replaced by nC atoms, respectively. The formation energy for 2C at Al, 2C at N, 4C and 6C doped AlN systems were gained as -1.6 eV, -2.83 eV, -3.96 eV and -4.32 eV, respectively. The negative formation energies indicate that, C atom incorporation in AlN lattice is thermodynamically favourable and stable C-AlN hybrid systems can be synthesized [36, 49].

CONCLUSION

The structural and opto-electronic parameters of carbon C atom-doped single layer AlN systems were investigated using first-principles DFT. The C atom concentration was varied from 6.25 % to 18.5 % (i.e. From two to six C atoms in 32 host atoms) and their effects were determined. Through electronic structure calculations, it is found that, C atom substitution in monolayer AlN makes it display half metal/semimetal/conductor behavior, depending upon the number of C atom present in AlN lattice. When two C atoms replaced Al atoms in AlN lattice, some impurity states appeared at the Fermi level, thereby making half metal material. When two C atoms replaced two N atoms in AlN layer, it displayed semimetal property having almost negligible band gap. Upon substituting 4 C atoms in AlN layer, a conducting AlN material was achieved having band gap of ~0.7 eV in its electronic structure. Similarly, when 6C atoms replaced a whole AlN ring, a semiconducting C-AlN hybrid material was obtained having 2.2 eV band gap in its electronic structure. Using random phase approximation (RPA) technique implemented with density functional theory (DFT), the optical absorbance and reflectance parameters was investigated for pure and C doped AlN systems. For pure AlN system, we have zero absorption quantity in between 0-8 eV energy and have almost negligible static reflectivity parameter. However, when various C atoms were placed in AlN lattice, the optical absorbance is improved in low lying energy range, suggesting a red shift towards visible region of spectrum. The static reflectivity parameter was also improved after C atom substitution and reflectivity is reduced in higher energy range.

In general it can be summarized that, by incorporating C atoms in AlN layer, opto-electronic behaviours of AlN systems can easily be modified and functional hybrid C-AlN systems can be synthesized, those can be utilized for real opto-electronic device applications.

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