

Doping of 3d-Transition Metals on Monolayer of Graphene and Borophene



Keshav Dev, Swasti Saxena, Ankit K Srivastava, B.S Bhadoria, Suneel Kumar

Abstract: We Study the doping of various metallic 3d transition metal (TM) atoms like iron (Fe), Cobalt (Co), Copper (Cu) and Nickel (Ni) on monolayer of the borophene and graphene. These 2D layers show energy dispersion and metalloid properties because its band gap is very less or near to zero. We explored borophene is semi-metallic with the titled Dirac cone and graphene is semi metallic whose conduction and valence bands meets at Dirac cone. We analyzed the adsorption of 3d transition metal (TM) on the 2D layers through density functional theory (DFT) based calculations. In this paper, we observed the most suitable and acceptable adsorption site for each adatom, and calculated the binding energy per atom, density of states and magnetic moment of resulting borophene and graphene-adatom system. Here, we find that Nickel (Ni) is perfect as electron doping and iron (Fe) is the most effective for magnetically doped borophene. In the case of graphene we find that Co is most suitable for magnetically doping and Cu is best for electron doping.

Keywords: Borophene, Density Functional Theory (DFT), Graphene, Transition metal.

I. INTRODUCTION

Graphene has become an interesting element to catch attention from the researchers. Monolayer graphene created a new interest in the area of two-dimensional (2D) materials in the condensed matter physics [1]. Based on its 2D structure, Graphene have inspired many scientists to provide a new future in the field of electronic, magnetic and photonic science based on its fascinating properties [2], [3]. Graphene has remarkable electrical properties because of its high electron mobility at ambient condition. Graphene is an atomically thick 2D material and transition metal chalcogenide (TMDs) are being researched with great effort to use their exceptional electronic properties and magnetic properties [4], [5] Graphene is an one atom layer thick carbon sheet, has many marvellous properties [2], such as great intrinsic mobility, no bandgap, zero effective mass, high

electrical and thermal conductivity [6], [7], stiffness, magnetic and optical properties. On the other hand, borophane, considered a ‘wonder material’ which has revolutionise batteries, photovoltaics, electronics, sensors applications, and quantum computing. Borophene is a single layer of boron atom with the bonding of atomic hydrogen, has been recently synthesized on a silver (Ag) substrate film prepared in ultrahigh-vacuum [8]-[14]. It is super-strong and super-flexible. Borophane is not just stable at standard temperatures and air pressures, but also has high mechanical strength, flexibility and superconducting properties. Before borophane comes in the limelight, there was borophene, an analogue of graphene, which was very popular as a wonder material. The investigation for other graphene like two-dimensional materials always attracted many scientists groups to predict in the 1990s and then boron atoms took attention because it can form a monolayer through computer simulations. However, it was synthesised only in 2015 [10]. Many studies have proved that borophene is a stronger, lighter and more flexible than graphene but borophene has a disadvantage that it can only present inside of an ultrahigh vacuum chamber and because of this limitation it can practically use outside of the lab. But Now, Mark Hersam at Northwestern University in Illinois and his team have given a solution for overcome this problem. They deposited atomic hydrogen onto the surface of metal decorated borophene to develop borophane. The outcome proved that the hydrogen storage capacity has been influenced due to the metal atom decoration and light mass of the boron element. As resultant they found four phases of borophenes after synthesis which has been reported as 2-Pmmn, $\beta 12$, $\chi 3$ and honeycomb phases [15], [16]. These all phases are metallic and semi metallic in nature. Different experimental and many theoretical studies on borophene has been shows the excellence superconducting properties, mechanical properties, lattice thermal conductivity, electronic structure, optical properties, surface reactivity and atomic adsorption [8]. Borophene also shows some unique and excellent physical and chemical properties such as the 2-Pmmn phase of borophene has a unique buckling structure with triangular arrangement, where the boron atoms can be classified into two category, “peak” and “valley. The main problem of ‘the borophene’ is that there is no way to produce it in large quantities yet but researchers are working hard for this direction. Graphene inherently have no magnetic properties but with the doping of some transition metals it shows small magnetic moment like hydrogen (The exert force can be driven by the magnet and the direction of the force will be the direction of the magnetic moment).

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This doping of hydrogen atom can made graphene layer magnetically active and hydrogen atom transfers its magnetic moment to graphene layer [6], [17]. There is many other doping like Fe, Cu, Co Ni etc which can also exert magnetic moment to the graphene layers [7], [8]. The researchers provide an explanation for that during contraposition to greater not unusual magnetic substances consisting of iron, nickel or copper, cobalt, wherein the magnetic moment generated with the aid of each atom is placed within a few tenths of a nanometre, the magnetic second induced within the graphene by every atom of hydrogen extends several nanometres, and also presentations a modulation on an atomic scale. A perfect depiction of the electronic properties of these elements can be assembling by their band structures and the temperature dependence of the electronic conductivity. As we know that transition metals have partially filled energy bands in their metallic states, and Fermi level intersects at a partially filled energy band (Figure 1). When temperature applies on metals it's become very poor conductors (almost behaves like insulators) because of lattice vibrations. The moving valence electrons are scattered as a result of this mechanism. At higher temperatures, semiconductors and insulators with filled and empty bands, on the other hand, become better conductors because some electrons are thermally driven to the lowest vacant band. The distinction between insulators and semiconductors is arbitrary, because all semiconductors are insulators in terms of metal-insulator transitions. If the band gap (E_{gap}) of an insulator is less than around 3 eV, we call it a semiconductor. Single sheets of sp²-bonded carbon (graphene) and elemental Borophene are examples of semimetals with a band gap near zero. A semimetal, like a narrow-gap semiconductor, exhibits better conductivity at higher temperatures. [18], [19].

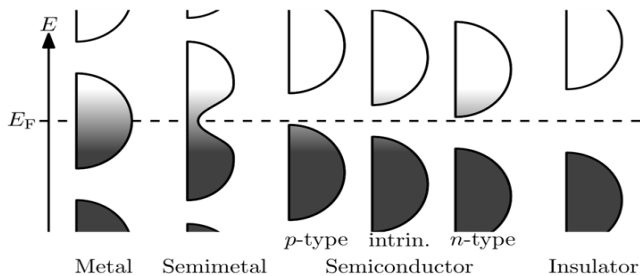


Figure 1: Density of available states of materials at Fermi energy level.

The electrical and magnetic characteristics of borophene and graphene following doping of 3d transition materials were calculated theoretically in this review. Then, as future applications, we'll concentrate on the physical qualities of borophenes and graphene, which will include mechanical, thermal, electrical, optical, and superconducting properties. Finally, we review the applications of metal ion batteries, hydrogen storage, sensors, and catalysts in hydrogen evolution, oxygen reduction, oxygen evolution, and CO₂ electroreduction reactions. Although the bulk allotropes of carbon and boron are very different, small clusters of these elements have a lot in common. The graphene-like structure was buckled and metallic, with a weak connection to the substrate. Two-dimensional (2D) materials have no bulk counterparts due to substrate-stabilized growth and frequently exist as single atomic layers. Although multilayer

creation is widely desired for structural and property tuning, it has yet to be achieved in the case of synthetic 2D boron, i.e. borophene [20]-[22].

II. THEORETICAL CALCULATION AND PREDICTION:

A. Computational Method

The ab initio calculations [23] of the system are performed using the Quantum ESPRESSO [24] for all DFT calculations. We use spin-polarized density functional theory with generalized gradient approximation (GGA). The exchange-correlation part of electron-electron interactions is treated within the generalized gradient approximation (GGA) as implemented as Perdew-Burke-Ernzerh (PBE). A plane wave basis set with an energy cut off of 540 eV is used. All the calculations have been performed with Monkhorst-Pack sampling of $[10 \times 10 \times 1]$ k-mesh. Atomic positions were relaxed with force tolerance limit of 0.01 eV/Å. To begin, the rectangular unitcells of 2-Pmmn borophene with two atoms and 8-Pmmn borophene with eight atoms per unit-cell were totally loosened. The optimised lattice constants for 2-Pmmn borophene are $a = 2.888$ Å, $b = 1.602$ Å, and for 8-Pmmn borophene, $a = 4.510$ Å, $b = 3.250$ Å, which are in good agreement with previously reported values as summarised in Table 1. The relaxed unit-cells are utilised to create 3 3 1 super-cells for 2-Pmmn borophene with 18 boron atoms and 2 3 1 super-cells for 8-Pmmn borophene with 48 boron atoms for 2-Pmmn borophene. To prevent spurious inter-layer interactions among the monolayers, a vacuum area of 20 Å is applied on each side of the super-cell. For the unit cells, we considered the k-grid density. Transition metal atoms are adsorbed at diverse sites on these relaxed super-cells based on geometrical aspects. All structures (with and without adatom) are fully relaxed until the force on each atom is less than 0.01 eV/Å with convergence threshold 10⁻⁸. In the other hand for graphene, We employed a density functional theory-based first-principles band computation technique. We employed Quantum ESPRESSO, a high-precision first-principles computation code based on DFT calculations. All computations were done nonmagnetically on a plane wave basis with a 500 eV energy cutoff. The graphene sheet's unit cell was designed with a 3 3 1 shape. The graphene's lattice constant was based on the calculated value. The spacing between graphene sheets is around 14.7 micrometres, and the gap between adatoms is approximately 7.3 micrometres. In the irreducible Brillouin zone, the final potential is constructed self-consistently from eigenstates at 24 sampling k-points (IBZ). We treated almost all 3d transition materials except the lanthanoids and noble gases as adatoms and carried out the calculation.

B. Band Structure of Borophene

2-Pmmn borophene is metallic in nature, as seen in Fig 2(a) and 2(b), whereas 8-Pmmn borophene exhibits an anisotropic Dirac cone-like dispersion, similar to graphene, with the Dirac point in the middle of the -X line.

Figures 2 and 3 illustrate the total density of states (DOS) for pristine 2-Pmmn and 8-Pmmn borophene.

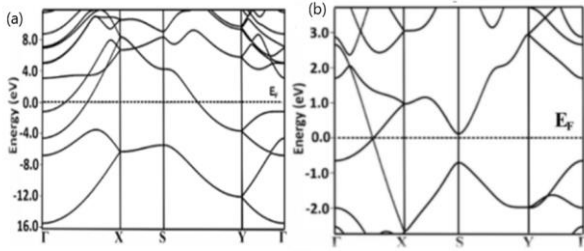


Fig 2: (a) band structure for 2 Pmmn borophene (b) band structure for 8 Pmmn borophene

C. Band Structure of graphene

The band structures of 2-Pmmn borophene (a) and 8-Pmmn borophene (b) indicate that 2-Pmmn borophene is metallic in nature, whereas 8-Pmmn borophene has an anisotropic Dirac cone-like dispersion, similar to graphene, with the Dirac point in the centre of the -X line. Figures 2 [25][26] illustrate the total density of states (DOS) for pristine 2-Pmmn and 8-Pmmn borophene.

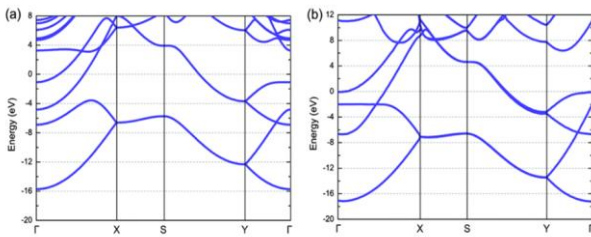


Fig 3: (a) band structure for graphene (b) band structure for 63/Pmmm graphene

D. Electronic Structure

Single adatom:

For adsorption on the surface of each borophene layer, we consider two distinct magnetic transition metal atoms (Fe/Ni). Single adatom adsorption in the specified unit cell results in doping concentrations of 5.58 percent for 2-Pmmn borophene and 2.06 percent for 8-Pmmn borophene, which are both within the experimental limits. On the basis of binding energy estimates, the most stable adsorption site is predicted among all possible adsorption sites. The binding energy is calculated as follows:-

$$E_{\text{binding}} = E_{\text{borophene}} + E_{\text{adatom}} - E_{\text{borophene+ adatom}} \dots\dots(I)$$

Where,

$E_{\text{borophene}}$ and E_{adatom} are the total energy of the pristine borophene monolayer and an isolated transition metal adatom, respectively.

$E_{\text{borophene+ adatom}}$ are the total energy of the relaxed borophene-adatom system.

Table 2 summarises the binding energy of several adatoms adsorbed at various sites on 2-Pmmn and 8-Pmmn borophene polymorphs. In 2-Pmmn borophene, Fe prefers the B3 site, whereas in 8-Pmmn borophene, it prefers the C site. The binding energy of the B3 site on Fe on 8-Pmmn borophene is very near to that of the C site, making it a likely place for adatom adsorption. In 2-Pmmn borophene, Ni is more energetically stable at the C site, while in 8-Pmmn

borophene, Ni is more energetically stable at the B3 site. Note that, contrary to our findings, T1 was found to be the most stable site for F and Ni adsorption in 2-Pmmn borophene in a previous study [27]. This discrepancy, we assume, is due to the fact that the B3 and C locations were not studied in their research. We have find that the B3 site has higher binding energy as compared to the T 2 site. [28][29].

Table 1 summarizes the borophene lattice constants a, b, and buckling height h.

S.N	Calculated			Reported		
	a(°A)	b(°A)	h(°A)	a(°A)	b(°A)	h(°A)
2-Pmmn	2.886	1.603	0.9635	2.863	1.615	0.912
8-Pmmn	4.512	3.252	2.185	4.524	3.257	2.181

Table 2: Binding energy per atom (in eV) for transition metal adatoms on 2-Pmmn borophene and 8-Pmmn borophene for all possible adsorption sites. The most stable site is the one with the highest binding energy.

Borophene	Atom	T1	T2	B1	B2	B3	C
2-Pmmn	Fe	0.116	0.182	0.123	0.169	0.217	0.180
	Ni	0.159	0.210	0.165	0.201	0.210	0.237
8-Pmmn	Fe	0.035	0.041	0.028	0.042	0.053	0.053
	Ni	0.055	0.065	0.051	0.065	0.067	0.065

Note: Bold values shows highest binding energy at the corresponding adsorption site in comparison to all other adsorption sites for that adatom. When we concentrate on the calculation for the crystal structure and energy dispersion, on 2-Pmmn and 8-Pmmn borophene, we can compute the adsorption of transition metal adatoms. Figures 1a and 1e show the six distinct adsorption sites for both borophene polymorphs. Table 2 shows how these are labelled: (a) above the centre of the hexagon in the upper layer (T1), (b) above the centre of the hexagon in the bottom layer (T2), (c) at the bond centre in the upper borophene layer (B1), (d) at the bond centre in the lower borophene layer (B2), (e) at the centre of the bond connecting the upper and lower borophene layer (B3), and (f) at the centre of the triangle (C). A 96x96x1 Monkhorst-Pack grid is used to determine the DOS (density of state) of virgin graphene in a primitive unit cell, which is dense enough to resolve the zero DOS at the Dirac point energy. For DOS calculations, an adsorbate atop a 4x4 supercell of graphene requires only a 24x24x1 grid to provide an overall sampling density similar to pristine graphene [4]. To estimate the Dirac point, the peaks in the DOS from weakly hybridised, low-lying sp² states can be compared to those of pure graphene (Fig. 3). The position coordinate of the adatom parallel to the surface is fixed for the calculation of adatoms at specified locations, while the coordinate normal to the surface is totally relaxed. During the relaxation of the other carbon atoms of the graphene sheet, one atom of the edge of the 3x3x1 configuration is fixed.

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We used 240 k-sampling points in the IBZ to do convergent calculations utilising the coordinate with convergent potential. We calculated a 3x3x1 graphene to get a final potential. Band structure and BZ of 3x3x1 graphene and borophene are shown in Figures 2 and 3. The adsorption energy was determined using the formula

$$E_{\text{bond}} = (E_{\text{graphene}} + E_{\text{adatom}} - E_{\text{total}}) \dots \dots \dots \text{(II)}$$

E_{bond} is the adsorbed atom's binding energy to the graphene sheet. The total energy of one sheet of graphene is E_{graphene} , whereas the total energy of an isolated adatom is E_{adatom} .

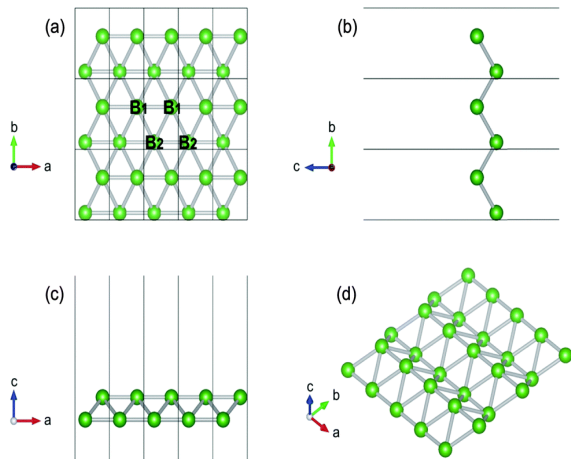


Figure 2: Structure of Borophene

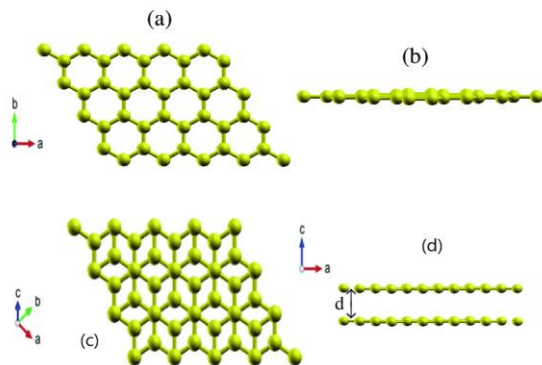


Figure 3: Structure of graphene

Table 3: The binding energy per atom ($E_b = -E_a$, in eV where E_a is absorption energy), the ratio of binding energy to bulk cohesive energy (E_b/E_c), the distance between the adatom and the nearest boron atoms (d_{ac} in \AA), the magnetic moment of isolated atom (μ_b), the magnetic moment of adatom-borophene system (μ_{ba}) for 2-Pmmn and 8-Pmmn borophene. Δq is the charge transfer.

Borophene	Atom	Favorite site	$E_b(\text{eV})$	$E_c(\text{eV})$	E_b/E_c
2-Pmmn	Fe	B3	0.2173	4.28	0.97
	Ni	C	0.2378	4.44	1.02
8-Pmmn	Fe	C	0.0532	4.28	0.61
	Ni	B3	0.0673	4.44	0.74

Borophene	Atom	Favorite site	$d_{ac}(\text{\AA})$	$\mu_a(\mu_B)$	$\mu_{ba}(\mu_B)$	Δq
2-Pmmn	Fe	B3	1.9	4.01	0.01	-0.2e
	Ni	C	1.93	1.99	0.01	0.80e
8-Pmmn	Fe	C	1.86	4.01	1.97	0.05e
	Ni	B3	1.87	2	0.01	0.89e

Table 4: We compute and compare the magnetic moment of the adatom–borophene system with that of the isolated atoms in this subsection. The number of unpaired electrons in the valence orbital of an isolated atom is the number of unpaired electrons in the valence orbital of Magnetic moment (in μ_B) comparison.

2D layers	Fe	Ni	Co	Cu
Graphene	2.13	0	2.252	0.002
2 Pmmn Borophene	0.01	0.01	1.431	2.274
8Pmmn Borophene	1.97	0.01	3.461	1.429

Table 3 summarises the magnetic moments of all the adatoms. When a transition metal atom adsorbs on a borophene monolayer, hybridization between the 4s- and 3d-orbitals of the transition metal atom is likely to occur, and the electron will transfer from the 4s- to the 3d-orbital. In their isolated state, Fe and Ni have magnetic moments of 4B and 2B, respectively. Because of the hybridization and total pairing of electrons, Ni adsorbed on 2-Pmmn borophene loses its magnetic feature completely. In addition to orbital hybridization, Fe adsorbed on 2-Pmmn borophene is expected to take some charges from the borophene monolayer (see negative charge transfer in Table. 3) and occupy all of its d-orbitals, yielding a magnetic moment of 0 B. However, even as an adatom on 2-Pmmn borophene, Co retains part of its magnetic properties, with the magnetic moment changing from 3 B to 0.7 B due to one unpaired electron. Due to hybridization, the magnetic moment of Ni vanishes after adsorption on 8-Pmmn borophene, while Co and Fe retain a finite magnetic moment of 0.9 B and 2 B, respectively, corresponding to zero, one, and two unpaired electrons. When travelling from Fe to Ni, i.e. moving right in the periodic table, the net magnetic moment for the adatom-8-Pmmn borophene system drops. After comparison from Table 5, we observed the change in magnetic moment for transition metals adsorbed on various 2D materials. This magnetic moment quenching on adsorption is similar to that observed in other two-dimensional materials such as 2-Pmmn borophene, graphene, and others.

III. RESULT AND DISCUSSION

At low temperatures, the 3d transition metal becomes spin polarised. For a few adatoms, calculations including spin polarisation are undertaken in some groups [30][31]. If the nonmagnetic state is one of the ground states, however, it is just as critical to calculate as the spin polarisation.

In other words, the nonmagnetic state is one in which the spin may be averaged, and it is the starting point for discussions of the ferromagnetic state at high temperatures. The electronic state in the nonmagnetic state is the initial stage in discussing the formation of a compound semi metal on graphene.

First-principles simulations are used to explore the electrical and magnetic characteristics of borophene functionalized via 3d transition metal (TM) atom adsorption. The findings reveal that 3d Transition metal atoms can be adsorbed on borophene with binding energies ranging from 5.9 to 8.3 eV. When Ti, V, Cr, Mn, and Fe atoms are adsorbed, the previously nonmagnetic borophene becomes ferromagnetic, and the magnetic moments are dominated by the TM atoms.

The Stoner criterion is used to discuss the genesis of ferromagnetism. Our findings suggest that by adsorbing 3d TM atoms to borophene, the magnetic characteristics of the compound may be efficiently controlled, which could have implications in spintronics and nanoelectronics.

When various adatoms are adsorbed at three adsorption sites, this figure depicts the most stable adsorption site and bond energy. The magnitude of the adsorption energy when each adatom is adsorbed to the most stable adsorption site is shown in Fig. 4. This study reveals that the H6-site is the most stable for transition metal elements. The B-site is the most stable for nonmetallic elements. The T-site is the most stable adsorption site for Co, where the valence electron number of the adatom is 1. Furthermore, the magnitude of each adatom's adsorption energy is particularly great for transition metal elements.

The adatoms of the nonmetallic elements in Cu have the highest adsorption energy. With an increasing number of d-electrons, the bond energy of transition metal elements tends to increase. Furthermore, when the number of Fig. 4 increases, the bond energy tends to decrease. Because the d-orbitals are moved down, the occupancy of d-electrons increases to more than half.

On metal element adsorption, the bond energy is quite high, yet this state is unstable because it is built from a confined non-bonding band at the Fermi level, and the Fermi level's number density of states (DOS (EF)) is very big. This demonstrates how simple it is to stick to the B-site. When the adatom is C, however, there are a few changes in the adsorption energy of the T-site and the B-site. The bond gap between graphene and the adatom is seen in table 3. ('The bond distance' refers to the distance between the graphene sheet's average position and the adatom.). The binding energy tends to decrease as the bond gap between the adatom and graphene is considerable.

The adatom exhibits physical adsorption-like bonding when the bond distance is large. The bond energy tends to increase when the bond distance is short. For an example, the bonding property is analogous to chemical adsorption.

Table 5: Co-graphene and Cu-graphene at B, H and T site and its magnetic moments shown in the given table.

adatom	migration	B site	H site	T site	moment
Co	0.73	1.88	2.61	1.83	0.92
Cu	0.43	0.23	0.7	0.23	0.00

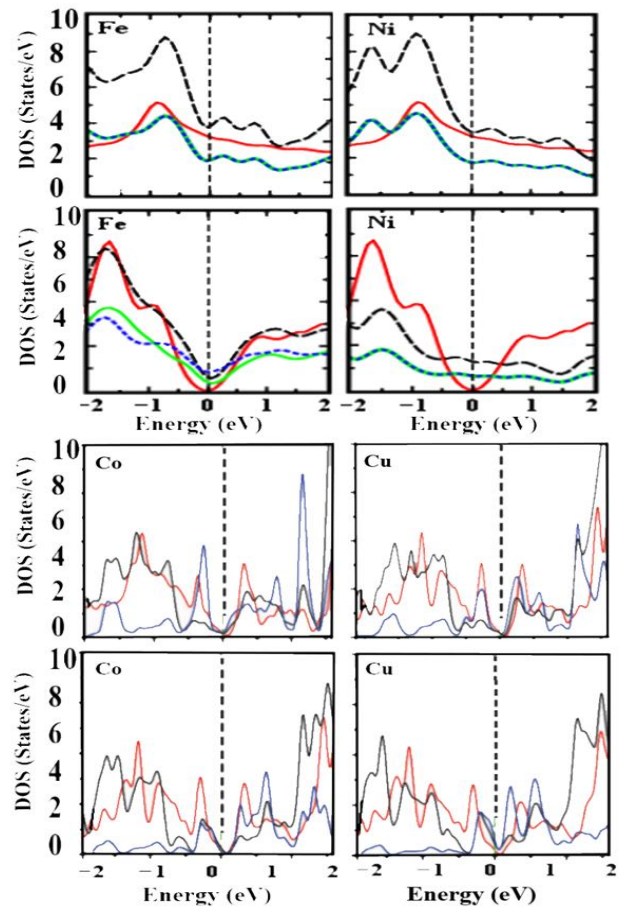


Figure 4: Total DOS and spin-polarized DOS of: (a and c) Fe adatom on 2-Pmmn and 8-Pmmn borophene (b and d) Ni adatom on 2-Pmmn and 8-Pmmn borophene, respectively. The DOS values are for the most favored site. Dashed black vertical line represents Fermi level (EF). Non-magnetic pristine borophene is converted into ferromagnetic by Fe on 8-Pmmn and Ni on 2-Pmmn, but the metallic and semi-metallic nature remains intact. (e and g) Co adatom on graphene monolayer (f and h) Cu adatom on graphene monolayer. Here, we can see that borophene is semi metallic with the titled Dirac cone like dispersion and graphene is semi metallic whose conduction and valence bands meet at Dirac cone. Density of states (DOS) of the 3d transition metal like Co doping on the monolayer of graphene in the presence of different electric fields shows very high magnetic moment. nanoparticles due to the strong electron transfer between Cu and Co, enhanced active surface area. The Dirac point was driven down towards the valence bands by the graphene's valence and conduction bands overlapping, and it appeared roughly 1 eV below the EF. The presence of a substantial electron density surrounding the EF shows that it is a conductor. Another band crossing point, i.e. Dirac point, was discovered by the current DFT calculation at the K-point, which is extremely close to the one illustrated in Figure 4. Interestingly, as seen in Figure 4, the d-orbital electrons of Co do not provide any substantial electron density in the overall DOSs.

As a result of the DOSs calculation, graphene features dominate in the Co structure material. Figure 4 (a-h) shows the band structures, DOSs, and individual components of the d-orbitals electron density of the TM (Fe, Co, Cu and Ni) atoms of the aforementioned materials. The most important discoveries about Co's material or electronic properties were discussed in this paper. Figure 4 (e-f) depicts the electronic characteristics of Co atoms intercalated in graphene, respectively. The intercalation of the Fe and Co atoms in borophene and graphene affected both the band structures and DOSs of BLG, and band structure studies revealed that the Dirac point is shifted down significantly from the EF. Although the VB and CB are overlapped onto each other in the Fe-borophene, the total DOSs calculations show that the electron density is extremely close to zero at the EF (like monolayer graphene), while Co-graphene shows metallic behaviour. The DOSs reveal that the electron has a small contribution to the total DOSs, showing that Co-graphene is a semi-metal. The DFT-D calculations revealed that VB and CB touch at EF, creating a Dirac Cone at the H-point in the graphene-Co bulk structure, and that VB and CB touch each other at the K-point around 1.3 eV above the EF. This suggests that in the bulk structure of graphene-Co, the graphene features 21 are prominent near the H-point. As a result, we may expect that the graphene-Co bulk structure is a Dirac material, while the 2D layer structure is a semi-metal with zero band gap. When Ni and Cu atoms intercalated in borophene and graphene materials, the Dirac points at K-point and H-point pushed down; see Figure 4. The total DOSs of borophene-Ni are close to zero at the EF, but graphene-Cu has a high electron density surrounding the EF, according to our calculations. As a result, there is no electron density at or near the Fermi energy level, indicating that borophene-Ni has semi-metallic behaviour. Due to the overlapping of VB and CB below the EF at the K-point in the layer structure BLG-Cu, a substantial electron density emerges in the total DOSs at the Fermi level, resulting in a conductor.

IV. CONCLUSION

Due to hybridization, the magnetic moment of Ni vanishes after adsorbing on 8-Pmmn borophene, but Fe retains a finite magnetic moment of 2B, corresponding to zero, one, and two unpaired electrons. When travelling from Fe to Ni, i.e. moving right in the periodic table, the net magnetic moment for the adatom-8-Pmmn borophene system drops. Table 4 compares the change in magnetic moment for transition metals adsorbed on various 2D materials. The structural, electrical, and magnetic properties of transition metal (Fe, and Ni) adsorbed 2-Pmmn and 8-Pmmn borophene complexes were examined in this study. The B3 site (middle of the bridge of upper and lower borophene atoms) is shown to be the most preferred location with greatest binding energy for most transition metal adatoms. Overall, the binding energy per atom for 2-Pmmn borophene is higher than for 8-Pmmn borophene, indicating that the former is more vulnerable to hosting metal adatoms. We also discovered that, with the exception of Ni on 2-Pmmn borophene, which has a uniform 2D growth pattern, all other adatoms are more likely to grow in a 3D island-like fashion. While Fe can accomplish full doping in 2-Pmmn borophene, we find that.

All three adatoms do electron doping in 8-Pmmn borophene. In both 2-Pmmn and 8-Pmmn borophene, Ni is determined to be the best choice for electron doping. The ground state electrical characteristics and geometries of Co and Cu adatoms adsorbed at four locations on graphene were calculated using density functional theory. The h-site (i.e. hole site) layout proved to be the most stable. For any particular element, this site is at least 0.4 eV more stable than other adsorption sites. Co adatoms tightly adhered to the graphene monolayer. This could imply that graphene has stronger sticking coefficients and diffusion barriers than other adatoms. Finally, for Co and Cu adsorbed at the h-site, the direct spin-up/spin-down band gaps at the K point. The electronic states of several Cu-graphene-based ferromagnets were investigated. Flat bands will be used to create Cu-graphene-based ferromagnets. For ferromagnetic interactions in Cu-graphene-based ferromagnets, the degeneracy of frontier flat bands and positive exchange integrals are important. We find that Ni is the most effective for electron doping; additionally iron (Fe) is the most suitable for magnetically doped borophene, while Co is best for magnetically doping and Cu is most suitable for electron doping for graphene.

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