iJRASET
International Journal For Research in Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 8 **Issue:** XII **Month of publication:** December 2020

DOI: https://doi.org/10.22214/ijraset.2020.32442

www.ijraset.com

Call: 08813907089 | E-mail ID: ijraset@gmail.com

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 8 Issue XII Dec 2020- Available at www.ijraset.com

Mg Decorated Boron doped Graphene for Hydrogen Storage: A DFT Method

Baliram Lone[1]
[1]*Nanomaterials Research Laboratory, Department of Physics, Vinayakrao Patil Mahavidyalaya Vaijapur, Dist. Aurangabad, Maharashtra 423701, India*

Abstract: ***First principles based DFT calculations performed to insight structural and electronic properties of Boron doped Magnesium atom decorated graphene sheet for application of hydrogen storage. The four H_2 molecules stably binds magnesium atom with Boron doped graphene sheet. The average binding energy extracted in the range-0.566 to -0.687 eV/H2.Partial density of states of complex system shows s and d orbitals of H_2 molecule and Mg atom at -0.1eV overlaps of main peaks indicates strong hybridizing and binding of s and d orbitals of H_2 and Mg atom respectively. HOMO & LUMO study shows stability of complex system. DOS investigation reveals the electronic density of states of complex system.***
Keywords: Graphene, Hydrogen storage, DFT, Boron doping, Magnesium

I. INTRODUCTION

In our daily life,there is a rapid increase in energy consumption to improve human development in terms of productivity and economic growth. Our goal is to replace the oil consumption by using new energy sources! The study of molecular hydrogen is alternative energy resource due to its vast applications in various fields [1-4]. Ensuring clean and efficient energy sources is one of the biggest challenges that we face in the 21st century.

With high energy conversion efficiency, zero pollutant emission, clean-burning product, rich in energy per unit mass, and most potentially abundant source, hydrogen energy is considered as the most clean and promising alternative energy source in the future [5].

To realize the Hydrogen Economy [6], the prime goal is investigating of safe, efficient and effective stores for H_2 gas, and replace current technologies based around the compression of H_2 as a liquid or as a gas using cryogenic. Recent, theoretical studies explained the poor capacity of H_2 adsorption on monolayer graphene surface. The theoretical results indicate, the adsorption energy (E_{ad}) of H_2 on graphene sheets is approximately 5 kJ/mol [1], which is far from the recommended E_{ad} (20-40 kJ/mol or 0.2-0.6 eV/Hydrogen molecule) for use of practical applications [7]. Therefore, enhanced adsorption energy of hydrogen on graphene could improve its uptake at room temperature [1].

Furthermore, theoretical results validate that a key factor leading to low H_2 adsorption capacity of pristine graphene [8] is weak binding between graphene sheets and H_2 atoms under ambient conditions.

The decoration of graphene (Gr) sheets is considered as one of the promising methods for hydrogen uptake improvement at ambient temperature [9,10].Transition metals such as palladium (Pd) [11], calcium (Ca) [12] , The adsorption of hydrogen on boron doped graphene indicates the hydrogen storage capacity increases by doping the boron atom [13]. The study of PtH_2systems absorbed on pristine and defective graphene explored the role of A van der Waals interaction[14], vanadium (V) [15], titanium (Ti) [16], nickel (Ni) [17], iron (Fe) [18] and Aluminium [19] can be useful for this purpose.

The magnesium hydride considered as promising candidate for hydrogen storage materials due to its high hydrogen capacity [8],among these transition metals, palladium provides the best conditions for hydrogen storage due to high catalytic activity [8] and high affinity for hydrogen sorption [20]. Pd is five times cheaper than Pt and more electrochemically stable than other transition metal atoms such as Fe, Co and Ni [21].

To fulfill the demand of energy in vehicular system, one of the suitable way for production of renewable source such as hydrogen storage which is air pollution free promising candidate. We explored to achieve possibility of hydrogen storage for onboard application.

In this study, for the first time a novel structure of graphene sheets as Mg-doped graphene sheets with boron in the presence of Mg atom was proposed to improve the hydrogen storage. This serves as the main novelty of this study. During hydrogen adsorption, boron can increase the adsorption of dissociated hydrogen atoms; their simultaneous application could be beneficial. Boron doping is a feasible and practical method to alter the binding structure and enhance the adsorption performance of hydrogen.

©IJRASET: All Rights are Reserved

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 8 Issue XII Dec 2020- Available at www.ijraset.com

II. METHODS

We considered the model [23] and further quantum chemical calculations were applied by using density functional theory. We applied Vienna ab initio simulation code (VASP) [24-25] within PAW method. The exchange and correlation within local density approximation have been selected for our studied system. To interpret all the characteristics of molecular interactions no density functional theory describes it accurately, particularly Van der Waals (VdW) interactions [26-28]. The LDA method employed to study the physisorption energies of H_2 on CNT and graphene are in good agreement with experimental values [29-30].

However, the overestimate of the binding energy by LDA is compensated by the ignored van der Waals interactions [31-32]. The electron wave functions are expanded by plane waves with a kinetic energy cutoff of 450 eV to attain the required convergence. All of the self-consistent loops are iterated until the total energy difference of the systems between the adjacent iterating steps is less than 10^{-7} eV. The Brillouin zone is sampled by 5 × 5 × 1 mesh points in k-space based on Monkhorst-Pack scheme [33-35]. The effective range of the kinetic energy cutoff and the validity of the mesh density used in this calculation are determined by a convergence test using the theoretically estimated lattice constants of the pristine graphene, 2.46 Å. To avoid the interactions of adjacent slabs, the vacuum space of 20 Å is introduced for 4 × 4 supercell which contains 32 carbon atoms.

III. RESULTS AND DISCUSSION

A. *Characterization of Magnesium (Mg)*

We considered that Mg atoms distributed uniformly on graphene (Gr) sheet, However, the phenomenon of adsorption behavior of Mg on pristine graphene sheet investigated as mentioned in below equation. The adsorption energy (E_{ad}) of Mg on graphene (Gr) can be calculated as:

$$E_{ad-Mg} = E_{Mg/Gr} - E_{Mg} - E_{Gr} \quad (1)$$

Where $E_{Mg/Gr,}$ $E_{Mg,}$ and E_{Gr} are evaluated total energies of the complex Mg-decorated graphene sheet, isolated Mg atom and pristine graphene (Gr) sheet. The favorable adsorption site for magnesium atom on surface of Gr sheet have centre of a hexagonal ring. However, using above formula 1, the adsorption energy (E_{ad}) of Mg on graphene ($E_{ad\text{-}Mg}$) is calculated and it is reported -2.88 eV.

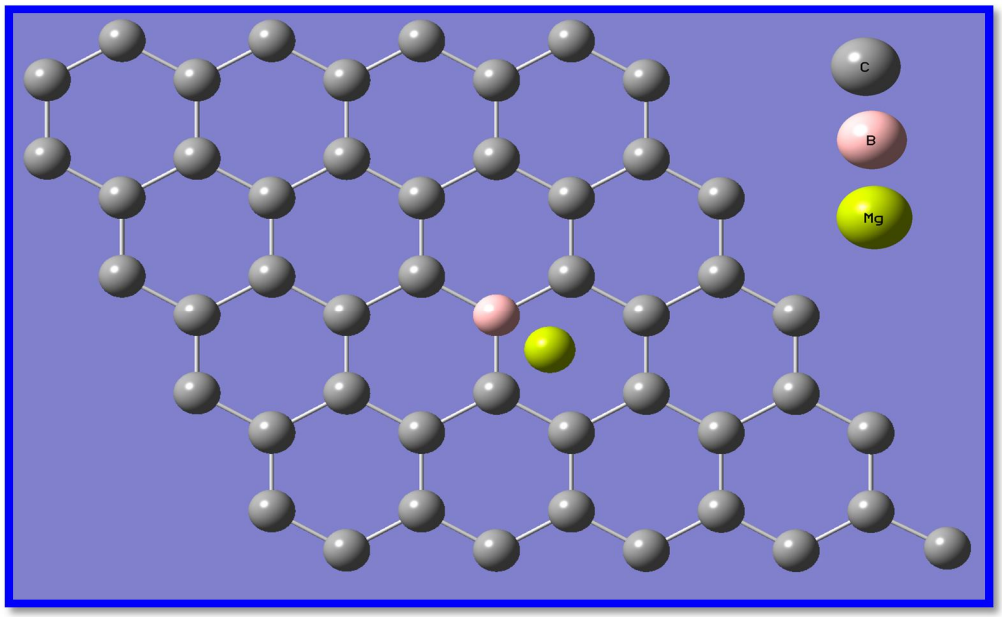


Figure 1. The Mg decorated stable graphene sheet with Boron doping atom.

However, the cohesive energy of complex system in solid phase of Magnesium found -4.26 eV/atom is greater than evaluated adsorption energy of Magnesium atom on pristine graphene sheet.

It implies that the magnesium atoms forms cluster. We introduce Boron atom to 4x4x1 graphene supercell, to achieve stable and uniform decoration of magnesium atoms on Gr sheet. The mechanism of adsorption energy (E_{ad}) of Mg on Boron doped graphene sheet is evaluated by

$$E_{ad-Mg} = E_{Mg/B/Gr} - E_{Mg} - E_{B/Gr} \quad (2)$$

©IJRASET: All Rights are Reserved

Where $E_{Mg/B/Gr}$,E_{Mg} and $E_{B/Gr}$ is total energies of complex system of the Mg decorated B doped graphene, isolated Mg atom and B doped graphene sheet respectively.

Under study, system is fully relaxed to achieve stable configuration stable configuration. The Mg atom tends to stay top site near the boron (B) atom as shown in figure 1. The distance between Mg and B atom is found 1.154 Å. The distance C-C 1.523Å whereas the distance between Mg and C atom is 1.334 Å.

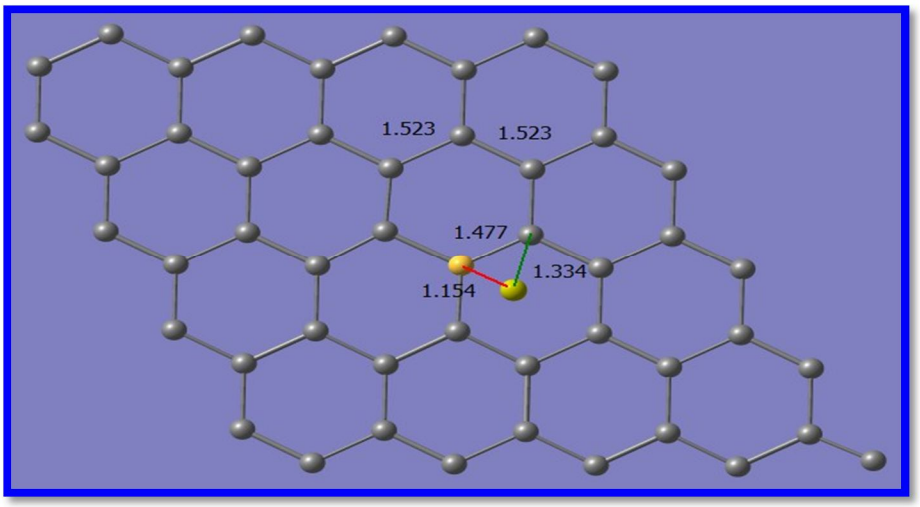


Figure 2 .The bond distance between Mg, B & C-C in Å

The investigated simulation result reveals the adsorption energy of Mg atom on Boron doped Gr sheet is -4.48 eV/atom is greater than bulk or complex solid phase magnesium cohesive -4.26 eV/atom.However,The formation of cluster of Mg atoms on Gr sheet can be prevented successfully by Boron doping process.

The magnitude of charges and distance between the centers of positive and negative charges i.e.diplole moment of the complex system (MgBC48) is 6.0771 Debye evaluated by B3LYP method using 6-31G basis set within Gaussian 09 suit [36].

B. Adsorption of Hydrogen on Complex system (Mg/B/Gr)

The complex system of Mg decorated boron doped graphene sheet investigated for the on board vehicular application of hydrogen storage. The adsorption of hydrogen (H_2) molecules on magnesium decorated graphene sheet summarized as:

After full relaxation optimized configurations of all H_2 molecules demonstrates in Figures 3 a-d (Top view).Figures 4a-d(side view) reveals the H_2 molecules prefers takes sites near to Mg atoms as well and vertical distance between first molecule and graphene sheet reported is 2.50 The other molecules exhibit same distance with the graphene sheet. The average bond length d_{Avg}=H-H is 0.925 Å which is elongated as shown in figure 3a, in gas phase bond length is 0.74 Å of the H_2 molecules.

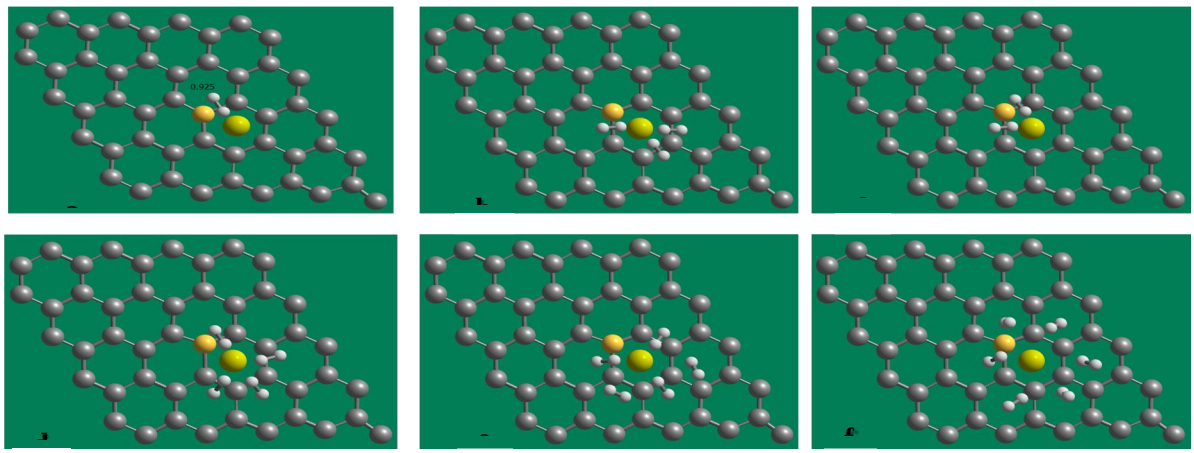


Fig.3 a-f. The optimized structures of H_2 molecules adsorbed on Mg/B/Graphene top view-I

©IJRASET: All Rights are Reserved

The side view-II of figure 4a-f implies, there is slight distortions in all configurations
particularly, in plane distortion to the graphene sheet. The lattice distortion in graphene layer [37] by means of adsorption of 3d-trasition metals confirms the reported slight distortions in Graphene sheet.
We know the stability H_2 molecules adsorbed on modified graphene sheet; we evaluated average adsorption energy of H_2 molecules using formula 3.

$$E_{ad-H2} = (E_{total} - E_{Mg/B/Gr} - nE_{H2})/n \quad (3)$$

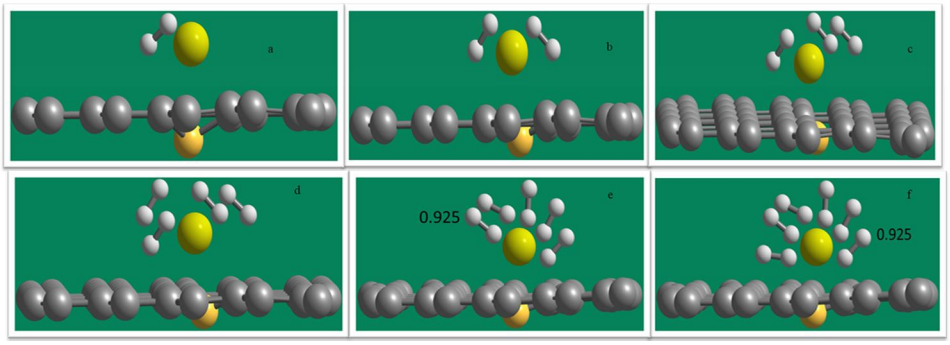


Fig.4 a-f. The optimized structures of H_2 molecules adsorbed on Mg/B/Graphene side view-II.

Serial Number	Number of H_2 molecules	Bond length of Mg/Gr in (Å)
1	$1H_2$	1.949
2	$2H_2$	2.296
3	$3H_2$	2.412
4	$4H_2$	2.225
5	$5H_2$	1.996
6	$6H_2$	2.249

Table 1 optimized bond lengths of the Magnesium decorated graphene (Mg/Gr) sheet for one to six adsorbed hydrogen molecules per Mg atom.

The extracted values of bond lengths in Å of graphene sheet for one to six hydrogen molecules per Mg atom are tabulated in table 1.The The extracted data shows there is continuous increase in bond length, when hydrogen molecules adsorbed on Mg decorated Gr sheet upto three hydrogen molecules afterwards slightly smaller in the fourth configuration (2.225Å in $4H_2$) ,fifth configuration (1.996 Å in $5H_2$),However, we increased adsorbed number of hydrogen molecules on surface of Mg decorated Gr sheet, But slightly increase in bond length is observed at sixth configuration (2.249 Å in $6H_2$).

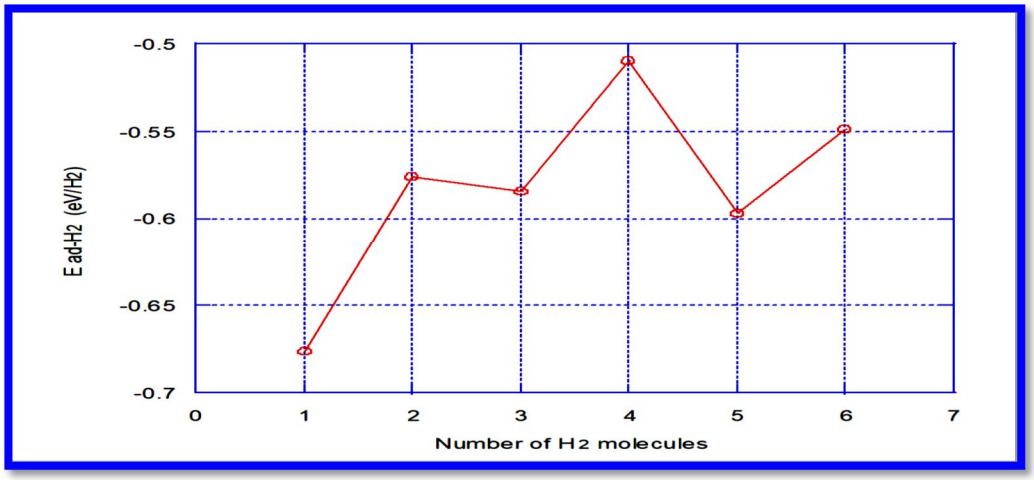


Figure 5. The average adsorption energies of hydrogen molecules on graphene sheet.

©IJRASET: All Rights are Reserved

The average adsorption energies of hydrogen molecules on graphene sheet shown in fig.5.from the plot highest value of adsorption energies is observed at $4H_2$ molecules, due to the Van der Walls interaction between the H_2 molecules and surface of the graphene [38]. Experimentally the 70% of adsorbed hydrogen is chemisorbed due to adsorption of hydrogen atoms.Then,how hydrogen molecule dissociate the on the surface of boron doped graphene? To overcome this, we used the NEB method to find the MEP of the hydrogen molecule dissociation on the surface of the B doped graphene[39].

After optimization of complex system considered, we able to evaluate the H-H and C-C bond lengths about 0.925 Å and 1.423 Å,respectively.The obtained values were compared with experimental values for H-H bond lengths is 0.74 Å [40] and 1.423 Å [41] for C-C bond lengths respectively.

1) *Properties of Mg on Hydrogen Storage:* To investigate the phenomenon of magnesium atom influence, on hydrogen storage mechanism of proposed study. we characterize interactions among Mg atom with graphene and hydrogen (H_2) molecules. Our results imply that, the boron atom accept charge from carbon atoms and increases adsorption energy (E_{ad}) of magnesium atom on Gr sheet due to presence of available empty p orbitals. However, the Mg atom can adsorb stably as well.

We investigated partial density of states of complex system $1H_2$/Mg/B/Gr as depicted in figure 5.

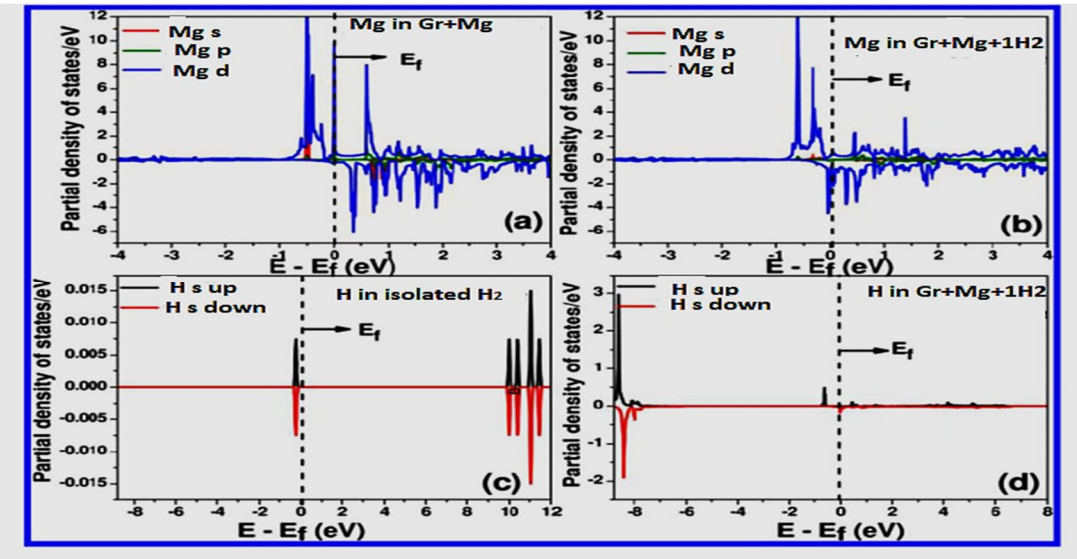


Figure 6. Partial density of states (PDOS) $1H_2$/Mg/B/Gr complex system.

It is observed that, s and d orbitals of H_2 molecule and Mg atom at -0.1eV depicts overlaps of main peaks. It indicates that strong hybridizing and binding of s and d orbitals of H_2 and Mg atom taking place.

There is a small amount of charge transfer the σ bonding of hydrogen molecule to d orbitals of magnesium atom. Simply, we studied the phenomenon of Mg influence atom on the process of hydrogen storage. Computational analysis performed, to reveal the interaction between Mg atom with Gr and H_2 molecules. The Boron (B) atom can accept charge from carbon (C) atoms and enhance adsorption energy (E_{ad})of Mg atom on the surface of graphene sheet due to its empty p orbitals. However, the Mg atom can adsorb stably as well.

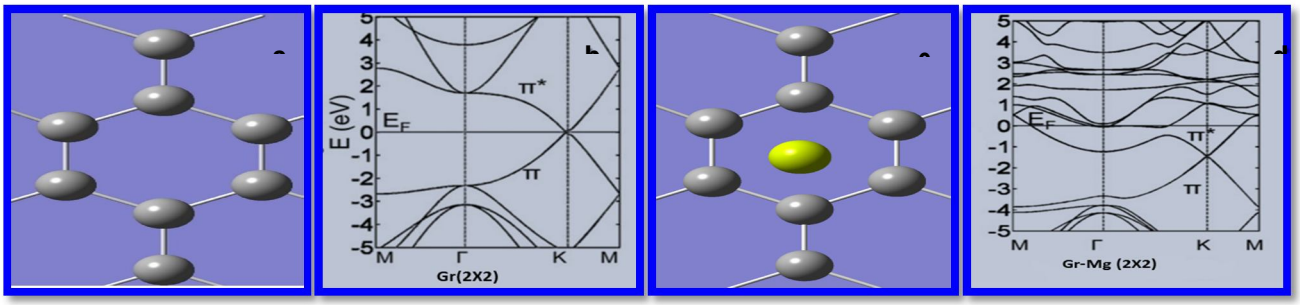


Figure 7.Gr (2X2) and Mg decorated Gr (2X2) with periodic boundary condition.

The above figure 7 shows denser coverage in Gr (2X2) and Mg decorated Gr (2X2) with periodic boundary condition.

©IJRASET: All Rights are Reserved

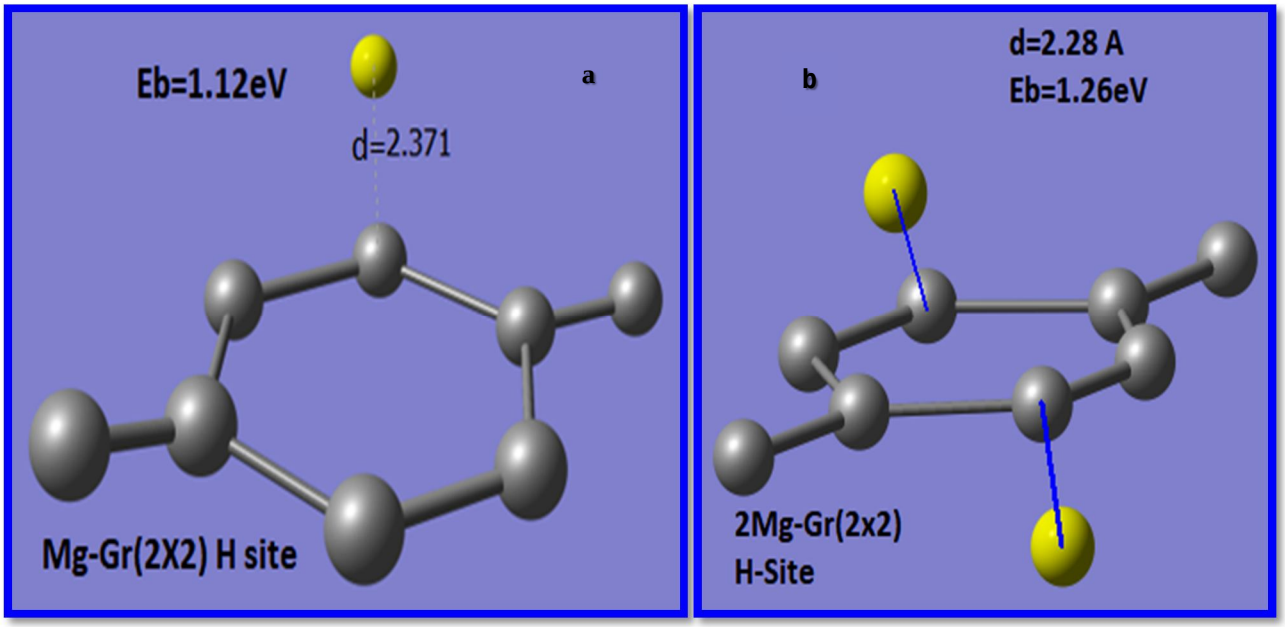


Fig.8.The optimized structure of single Mg atom (a) and double Mg atom (b) adsorbed on the H site of the (2X2) cell of graphene Mg -Gr(2X2).

Figure 8 indicates the optimized structure of single Mg atom (a) and double Mg atom (b) adsorbed on the H site of the (2X2) cell of graphene Mg -Gr(2X2).
If Mg adsorbed on one side the adsorption energy found 1.12 eV, however the Mg atom adsorbed on both side it is 1.26 eV, it is increased.

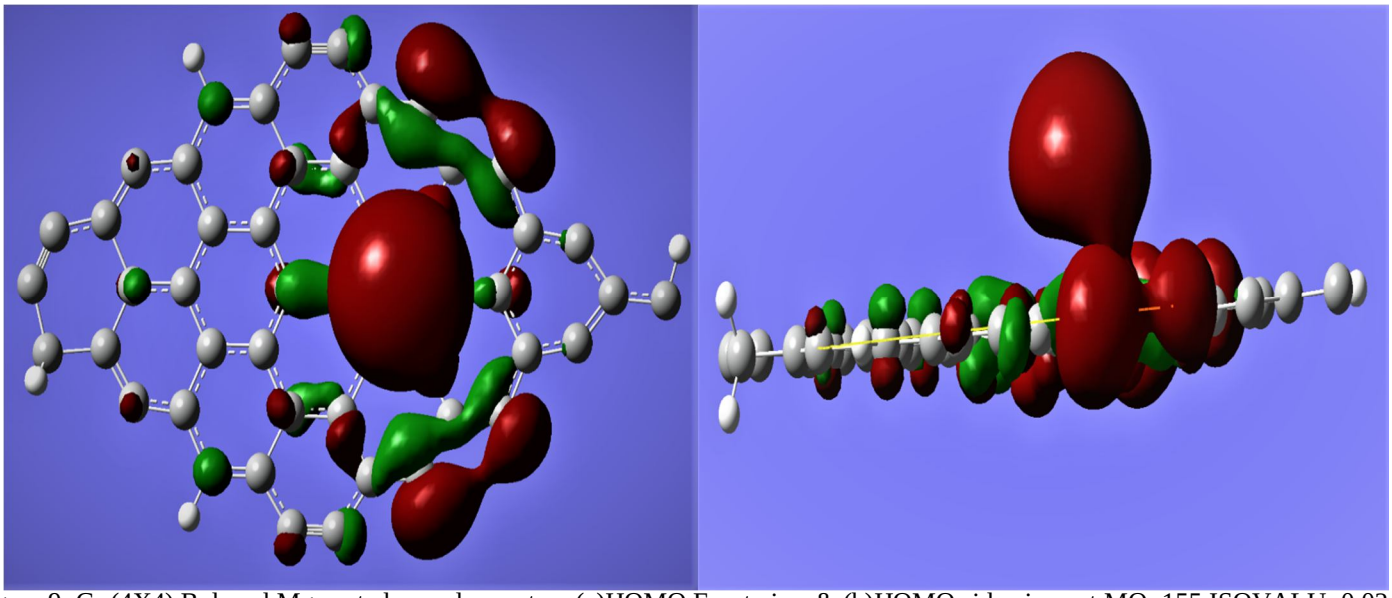


Figure 9 :Gr (4X4) B doped Mg coated complex system (a)HOMO Front view & (b)HOMO side view at MO=155;ISOVALU=0.02

Figure 9 shows (a) HOMO front view & (b) HOMO side view of the graphene (4X4) with boron doped Mg coated complex system. The computed HOMO value of complex system is -0.19997 eV. The highest occupied molecular orbital (HOMO) inferred properties like prediction of the strength and stability of the complex system [42].Fig.9 includes 155 molecular orbitals with fixed isovalue at 0.02.To evaluate HOMO-LUMO of Gr (4X4) B doped Mg coated complex system, all calculations performed by B3LYP/6-31G scheme within DFT using Gaussian 09 code[36].

©IJRASET: All Rights are Reserved

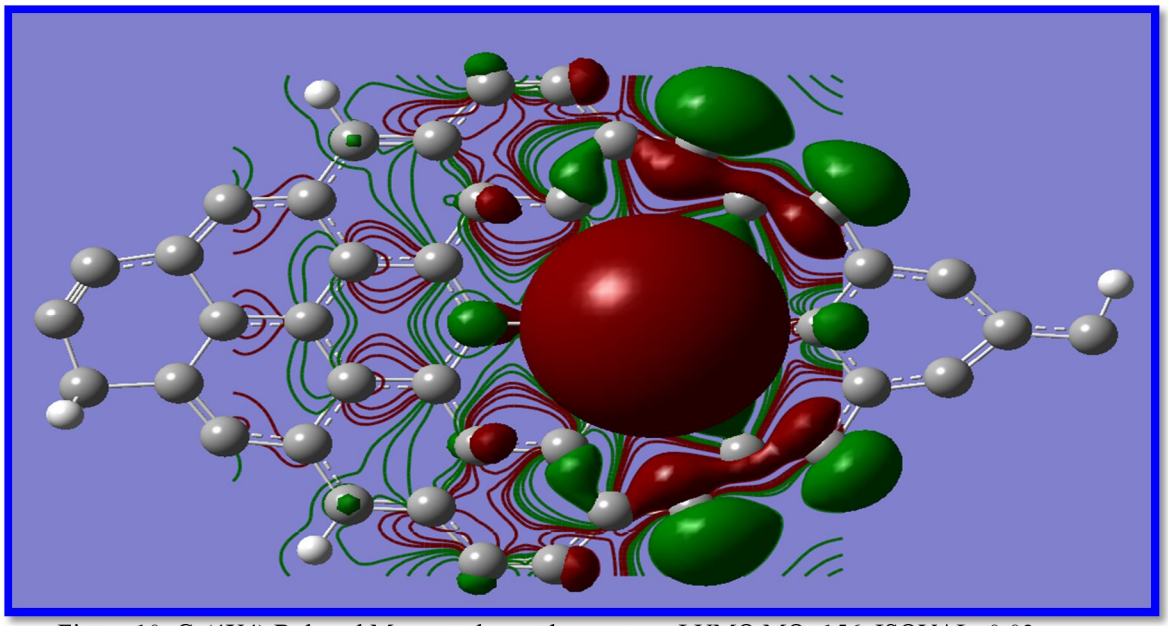


Figure 10: Gr(4X4) B doped Mg coated complex system -LUMO MO=156 ISOVAL=0.02

Figure 10 shows the lowest unoccupied molecular orbits (LUMO) for complex system of Gr(4X4) with Mg doped atom.The computed LUMO value of complex system is -0.17308 eV. The highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) of Gr(4X4) B doped Mg coated complex system displayed in figure 9 and Figure 10 respectively. The HOMO-LUMO surfaces play crucial role because these orbitals mainly participate in the interaction with other molecules in the complex system considered. From figure 9 and figure 10 we inferred that HOMOs are contributed by π orbital of graphene and LUMOs [43] are formed by s atomic orbitals of Mg. The HOMOs–LUMOs [Fig.9,Fig.10] both possess negative energy eigen values ,it confirms the formation of clusters which leads to stability of the complex system.

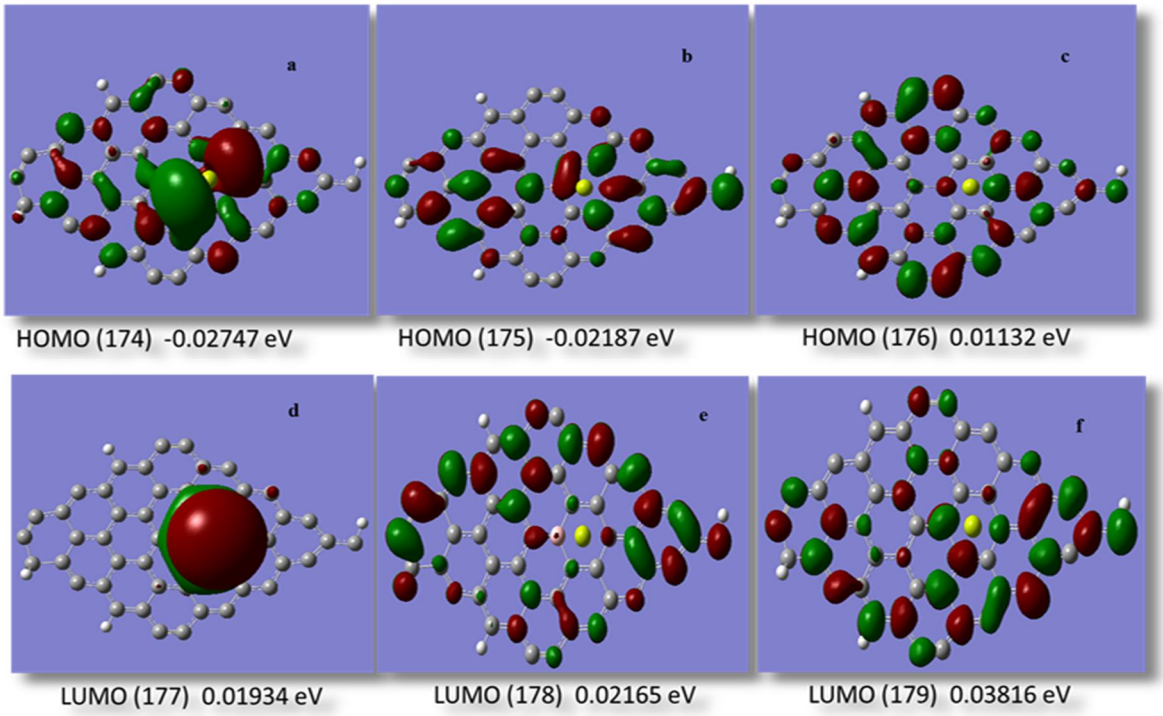


Figure 11(a-f): The mechanism of formation of Boron doped Mg decorated Gr(4X4) complex system HOMO-LUMO MO=174-179 ISOVAL=0.02.

©IJRASET: All Rights are Reserved

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 8 Issue XII Dec 2020- Available at www.ijraset.com

We inferred from above fig.11(a,b) that HOMO (174) -0.02747eV and HOMO(175) -0.02187eV represents negative electron density values due to contribution of Boron doped 2p orbitals and π orbital of graphene. There is distinct crucial role of boron which doped to graphene. Fig.11(c) clearly shows the only Boron atoms are involved in the mechanism of HOMO formation with contribution of values 0.01132eV. The S atomic orbitals of Mg are responsible for formation of LUMOs in complex system considered. Fig11(d,e,f) indicates increases of LUMOs Positive electron density values. One can inferred that HOMO and LUMO levels shift down and up with increase in size of the aggregated clusters, results in increase HOMO-LUMO energy gap. This favours the decrease in reactivity of the complex system. However ,increase in stability of complex system is observed.

The calculated HOMO (fig.9)-LUMO (Fig10) electron density energy gap of Gr(4X4) B doped Mg coated complex system are -0.19997 eV and -0.17308 eV respectively. This implies that there is -0.02689eV diffrerence in energy gap. We inferred from HOMO-LUMO that due to strong potential of B doped graphene the electron density is accumulated around carbon atoms of the complex system. The explored phenomenon of accommodation of the HOMO-LUMO states on B doped graphene surface signifies there is strong interaction between two interacting molecule species is observed [44-45].

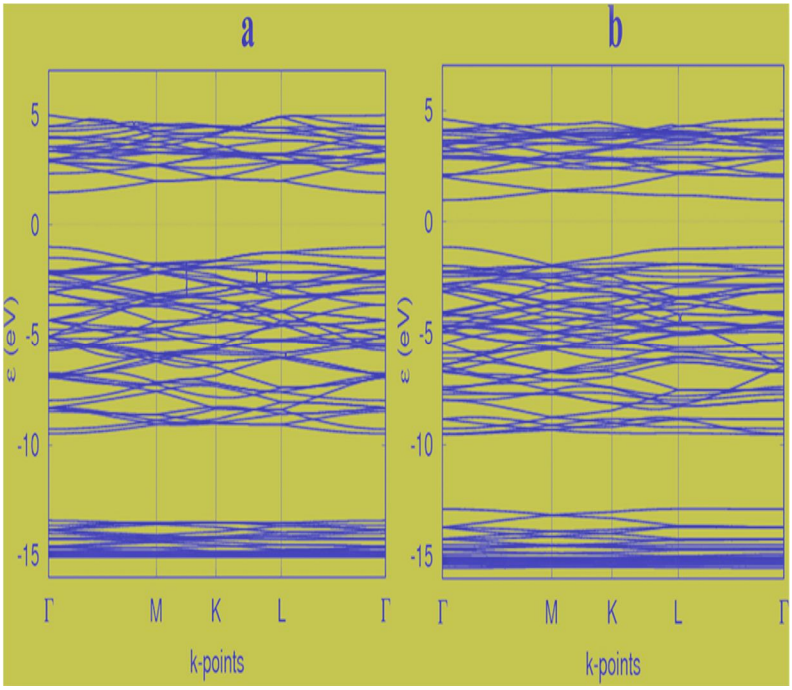


Figure 12.The calculated band structures at high symmetry k-points for complex system of B doped mg decorated graphene sheet. Gr-B-Mg configuration 1 (a) , Gr-B-Mg configuration 1 (b) .

The figure 12 indicates band structures at high symmetry k-points for complex system of B doped mg decorated graphene sheet. Gr-B-Mg configuration 1 (a) Gr-B-Mg configuration 1 (b).

In Fig.12 a,b. Gr-B-Mg configuration 1 and 2 reflects interaction taking between boron doped Gr by Mg atom decoration.

The complex system considered at the high symmetry Γ point, there is energy band gap of -0.1eV this decreases to -0.02689eV at M point. The energy band gap at K point is decreased to (fig.12) zero.These results are good aggrements with Fig.6 Partial density of states (PDOS) $1H_2$/Mg/B/Gr complex system [46-47].

IV. CONCLUSIONS

The quantum chemical analysis performed by using DFT within first principles method applied to complex system for hydrogen storage application. Our investigation suggests that Boron doped graphene with magnesium decoration achieved a uniform and stable decoration of individual B atoms on graphene sheet by Mg decoration. Our simulated data shows, there is $6H_2$ molecules modified system can absorb with adsorption energy (E_{ad}) in the range between -0.510 to 0.676 eV/H_2. In the complex system, magnesium atom acts bridge linking H_2 and Gr, due to which improves adsorption capacity of Gr sheet for H storage. Our findings enable excellent 2D Nanomaterial for hydrogen storage with vast outstanding potential.

©IJRASET: All Rights are Reserved

V. ACKNOWLEDGEMENTS

The authors are grateful to the financial support from department of science and technology (DST), New Delhi, India, under FAST TRACK SCHEME for YOUNG SCIENTIST, GRANT No. **SR/FT/LS-020/2009**(OYS 2009).The methodology development in this research work was supported by University Grants Commission (**Grant No. F 5-48/2013-IC**), New Delhi, India.

We Acknowledges departmental personnel from, Nanomaterials Research Laboratory at department of Physics, Vinayakrao Patil Mahavidyalaya, Vaijapur, Maharashtra., India, for their support in using their resources.

REFERENCES

[1] M. Hirscher, Handbook of Hydrogen Storage: New Materials for Future Energy Storage, Wiley-VCH Verlang GmbH & Co. KGaA, Winheim,2010.
[2] Jain, I. Hydrogen the Fuel for 21st Century. Int. J. Hydrogen Energy 2009, **34**, 7368−7378.
[3] R. B. Gupta, Hydrogen Fuel: Production, Transport, and Storage, CRC press, Boca Raton 2009.
[4] Momirlan, M.; Veziroglu, T. N. The Properties of Hydrogen as Fuel Tomorrow in Sustainable Energy System for a Cleaner Planet. Int. J. Hydrogen Energy 2005, **30**, 795−802.
[5] Schlapbach L, Züttel A. Hydrogen-storage materials for mobile applications. Nature. 2001;**414**(6861):353-358.
[6] Jonathan W. Steed, Jonathan W. Steed, Karl J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, Wiley-VCH Verlag GmbH, Boschstr 2007.
[7] Geim, A. K., Novoselov, K. S., The rise of graphene. Nature Materials 2007,**6**, 183-191.
[8] Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A., Electric Field Effect in Atomically Thin Carbon Films. *Science* 2004, **306**, 666-669
[9] Zhang J; Li ;Wu Y; Guo X; Ye J; Yuan B;Wang S and Jiang L, Recent advances on the thermal destabilization of Mg-based hydrogen storage materials. RSC Advances,2019,**9**,408-428.
[10] Lobzenko I.,Baimova J.,Krylova K. Hydrogen on graphene with low amplitude ripples: First-principles calculations, Chemical Physics ,2020,**530**, 110608.
[11] Hauser, A. W.; Schwerdtfeger, P. Methane-Selective Nanoporous Graphene Membranes for Gas Purification. Phys. Chem. Chem.Phys. 2012, **14**, 13292−13298.
[12] Hoonkyung Lee, J. I., Marvin L. Cohen and Steven G. Louie, Calcium-Decorated Graphene-Based Nanostructures for Hydrogen Storage. Nano Lett 2010, **10** (3), 793–798.
[13] Zhou Y.G., Zu X.T., Gao F., Nie J.L., Xiao HY. Adsorption of hydrogen on boron-doped graphene: A first-principles prediction. Journal of Applied Physics. 2009;105(1):014309.
[14] Lopez-Corrala I., Pirizc S., Faccioc R., Juane A., Avenaa M. A van der Waals DFT study of PtH2systems absorbed on pristine and defective graphene. Appl Surf Sci 2016;**382**:80-7.
[15] Pei P., Whitwick M.B., Sun W.L., Quan G, Cannon M., Kjeang E. Enhanced hydrogen adsorption on graphene by manganese and manganese vanadium alloy decoration. Nanoscale. 2017;**9** (12):4143-53.
[16] Mashoff T, Takamura M, Tanabe S, Hibino H, Beltram F,Heun S. Hydrogen storage with titanium-functionalized graphene. Appl Phys Lett 2013;**103**:013903.
[17] Ismail N, Madian M, Samy El-Shall M. Reduced graphene oxide doped with Ni/Pd nanoparticles for hydrogen storage application. J Ind Eng Chem 2015;**30**:328-35
[18] Sterlin M., Hudson L, Raghubanshi H, Awasthi S,Sadhasivam T, Bhatnager A, et al. Hydrogen uptake of reduced graphene oxide and graphene sheets decorated with Fe nanoclusters. Int J Hydrogen Energy 2014;**39**:8311-20
[19] Zhimin Ao, Dou S., Xu Z., Jiang Q, Wanga G. Hydrogen storage in porous graphene with Al decoration. Int J Hydrogen Energy 2014;**39**(28):16244-51
[20] Konda SK, Chen A. Palladium based nanomaterials for enhanced hydrogen spillover and storage. Mater Today 2015;**19**(2):100-8
[21] Sen D, Thapa R, Chattopadhyay KK. Small Pd cluster adsorbed double vacancy defect graphene sheet for hydrogen storage. A first principles study. Int J Hydrogen Energy 2013;**38**:3041-9
[22] Chen CH, Chung TY, Shen CC, Yu MS. Hydrogen storage performance in palladium-doped graphene/carbon composites. Int J Hydrogen Energy, 2013;**38**:3681-8.
[23] Li Y.,Mi Y ,Sun G. First Principle DFT study of hydrogen storage on graphene with La decoration,J.Material Sci.and Chem. Engineering 2015;**3**:87-94.
[24] Kresse, G. and Hafner, J. Ab Initio Molecular Dynamics for Open-Shell Transition Metals. Physical Review B, 993,**48**, 13115-13118.
[25] Kresse, G. and Furthmüller, J. Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors Using a Plane-Wave Basis Set. Computational Materials Science,1996,**6**, 15-50.
[26] Kresse, G. and Furthmüller, J. Efficient Iterative Schemes for *Ab initio* Total-Energy Calculations Using a Plane-Wave Basis Set. *Physical Review B*,1996,**54**, 11169-11186.
[27] Cohen, A.J., Mori-Sánchez, P. and Yang, W. Insights into Current Limitations of Density Functional Theory. *Science*, 2008, **321**, 792-794.
[28] Khantha, M., Cordero, N., Molina, L., Alonso, J. and Girifalco, L. Interaction of Lithium with Graphene: An *Ab initio* Study. *Physical Review B*,2004,**70**,125422.
[29] Lee, K., Murray, É.D., Kong, L., Lundqvist, B.I. and Langreth, D.C. Higher-Accuracy van der Waals Density Functional. *Physical Review B*,2010, **82**,081101.
[30] Perdew, J.P. and Zunger, A. Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems. *Physical Review B*, 1981,**23**, 5048-5079.
[31] Okamoto, Y. and Miyamoto, Y. *Ab initio* Investigation of Physisorption of Molecular Hydrogen on Planar and Curved Graphenes. Journal of Physical Chemistry B,2001,**105**, 3470-3474.
[32] Ao, Z., Jiang, Q., Zhang, R., Tan, T. ,Li, S. Al Doped Graphene: A Promising Material for Hydrogen Storage at Room Temperature. Journal of Applied Physics,2009,**105**, 074307

©IJRASET: All Rights are Reserved

[33] Leenaerts, O., Partoens, B. and Peeters, F. Adsorption of H_2O, NH_3, CO, NO_2, and NO on Graphene: A First- Principles Study. Physical Review B, 2008,**77**,125416.

[34] Cabria I., López M.J., Alonso J.A. Hydrogen storage in pure and Li-doped carbon nanopores: combined effects of concavity and doping. *J Chem Phys*. 2008;**128**(14):144704

[35] Monkhorst, H.J. and Pack, J.D. Special Points for Brillouin-Zone Integrations. Physical Review B, 1976,**13**, 5188- 5192.

[36] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 09 Rev. D.01*, Wallingford, CT, 2009.

[37] Lone B., Scheiner S., Kar T., Competition between carboxylic and phenolic groups for the preferred sites at the periphery of graphene–A DFT study.Carbon,2014,**80**: 405-418.

[38] Jhi S.H.,Kwon Y.K., Hydrogen adsorption on boron nitride nanotubes: A path to room-temperature hydrogen storage, Phys. Rev. B,2004,**69** ,245407.

[39] Wu X., Yang J., Hou J.G., Zhu Q. Defects-enhanced dissociation of H2 on boron nitride nanotubes. The Journal of Chemical Physics. 2006;**124(**5):054706.

[40] Kaye G.W.C., Tables of Physical and Chemical Constants. Longman, Harlow. 1995;**16** Edn:P-273.

[41] Ubbelohde A. R. Graphite and its Crystal Compounds. Clarendon, Oxford. 1960;31:P-5.

[42] Kato, K.; Iyama, T.; Tachikawa, H., Density Functional Theory Study of the Interaction of Magnesium Ions with Graphene Chip. Japanese Journal of Applied Physics 2011**, 50**, 01BJ01.

[43] Ganji M. D., Hosseini-khah S.M.,Amini-tabar Z.,Theoretical insight into hydrogen adsorption onto graphene: a first-principles B3LYP-D3 study, Physical Chemistry Chemical Physics 2015,**17** 2504-2511.

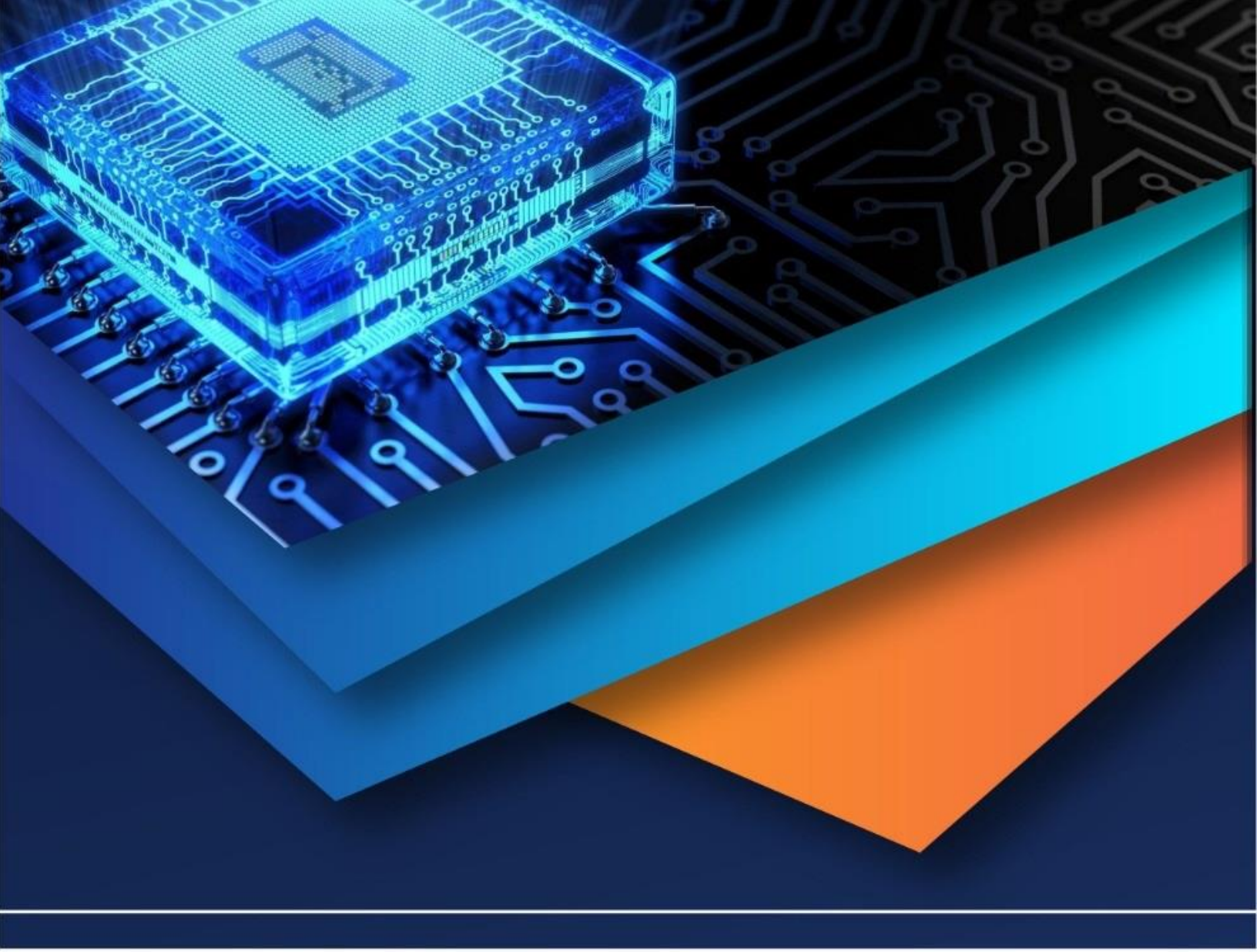
[44] Lone B.,Study of Arginine Amino Acid-Graphene Interactions. Advanced Science, Engineering and Medicine, 2019. **11**(3) 182-186.

[45] Nachimuthu S., Lai P.J., Leggesse E.G., Jiang J.C. A First Principles study on Boron-doped Graphene decorated by Ni-Ti-Mg atoms for Enhanced Hydrogen Storage Performance. Sci Rep. 2015;**5**:16797.

[46] Lebègue, S.; Klintenberg, M.; Eriksson, O.; Katsnelson, M. I., Accurate electronic band gap of pure and functionalized graphane from GW calculations. *Physical Review B* 2009, **79** (24), 245117.

[47] E. Beheshti, A. Nojeh, P. Servati, A first-principles study of calcium-decorated, boron-doped graphene for high capacity hydrogen storage, Carbon 2011, **49** 1561-1567.

©IJRASET: All Rights are Reserved



10.22214/IJRASET

45.98

IMPACT FACTOR: 7.129

IMPACT FACTOR: 7.429

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Call : 08813907089 (24*7 Support on Whatsapp)