

Edge Functionalization of Phosphorene with different Chemical Functional Groups

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ABSTRACT

Four allotropes of phosphorus namely, red, violet, white, and black phosphorus (phosphorene) named rendering to their entrance. Phosphorene few or maybe monolayer of black Phosphorus having bags of submissions in optoelectronics and electronic devices. Research is going to its belongings and device presentations has since understood exponential growth. So, we will investigating the tropical development in phosphorene study, moving up on the topics of Electronics and optoelectronics things and uses. We also confer upcoming development investigation and some tasks. We will also highpoint the phosphorene optoelectronic and electronic belongings resulting from phosphorene wrinkly construction which is different from graphene. The new the new properties of phosphorene will be moved design and protest of new devices but extra development joints on resolves to mechanical fences as surface degrading belongings and non-scalable manufacture methods. We temporary define the modern expansions of additional sophisticated project thoughts and application systems which report some of the tasks in black Phosphorus enquiry. This is predictable that attractive material remain to offer great breaks of research and evolution for predictable future. Different EDGE functionalization groups like at H, OH, COOH, and NH₂ are studied for chain extent.

Introduction

The Brandt, in 1969 was discovered first time phosphorus the 11th abundant element of earth crust (Lehman, 1958). White phosphorus is obtain as final product which is P₄ tetrahedral structure, having lone pair on the every phosphorus atoms. White phosphorus is precursor of organophosphorus when treatment with chlorine which is molecular form and the substrate used to introduce the substituents at phosphorus center (Basso et al., 2017). The red phosphorus allotrope is obtain when white phosphorus is heated that shows polymeric structure when few p-p bond breakage parent P₄ and formation of p-p new linkage between units which are different. In the presence of catalyst as iodine that further heated then this red phosphorus transformed into another phosphorus allotrope called black phosphorus (Nilges, Kersting, & Pfeifer, 2008). The polymerization degree of black phosphorus shared with red. This show the orderly the layered structures with the distance of interlayers is 3.11 Å (Hultgren, Gingrich, & Warren, 1935).

Likewise to graphite, phosphorene has a sheet construction which contains of a single component and can be simply extracted to single/few sheet arrangements (Gusmao, Sofer, & Pumera, 2017). The recent discovery of phosphorous as phosphorene 2D material having band gap nearly equal to 2 eV an important candidate for semiconductor show the higher ratio on/off carrier mobility of equal to 10⁴ at room temperature (Li et al., 2014). The recent interest in those materials which are layered graphene (K. S. Novoselov & Geim, 2007). Transition metal dichalcogenide also phosphorene due to their features (Wang, Kalantar-Zadeh, Kis, Coleman, & Strano, 2012). The reliable devices which having great performance definitely with high demands attempts the discovering the layered material which having important properties like carrier mobility. In the allotrope of phosphorous (Thurn & Kerbs, 1966). The phosphorene having natural band gap which is used for the formation of electronic devices as replacement may be suitable of silicone based devices. Phosphorene similar to graphene having puckered structure. Phosphorene also used for switching among conducting and insulating state due to its band gap (Liu, Neal, Zhu, Tomanek, & Ye, 2014). The great thermoelectric property having phosphorene used in thermoelectric devices. Their performance is that they

convert heat to electricity. The phosphorene which is alignment to electrical conductivity which is high and thermal conductance is poor boosted their thermoelectrically work. That is because of electron transport which is notable in phosphorene along the direction of armchair (Yang et al., 2015). Few experts show phosphorene capability as superconductivity with the transition temperature which is 3-16 K caused biaxial strain (Ge, Wan, Yang, & Yao, 2015). There are also something formed by researcher that when the temperature decrease from room as to 10 k then the carrier mobility rise to 5 factor (Liu, Neal, Zhu, Tomanek, et al., 2014). The researcher attention attracted by phosphorene recently due to the electrical and optical conductance. Due to these properties stabilizing highly dependent to production route that the phosphorene produced thin uniform and which should also multilayered (Yang et al., 2015).

Investigator predicted also that solvent which are polar and aprotic such as DMF and DMSO are possible solvent for the production of phosphorene which are thin Nano flacks. That production through this method defines new ways for black phosphorus mono layer mass production that utilize in optoelectronic and electronic devices. This is also concluded that the carrier mobility of phosphorene has up to $1000\text{cm}^2/\text{v}$ and at room temperature phosphorene transistor having off/on ratio up to 10^4 , 1-2. And also this material show the direct band gap in contrast with graphene which show application in all the devices which are based on light or those namely optoelectronic devices. (Li et al., 2014; Wood et al., 2014).

The systemic investigation of phosphorene on mechanical feature result show that phosphorene a super flexible that can stand having tensile strain 30 % may be 32% for Nano and multilayer respectively. The nature of phosphorene anisotropic was formed that direction dependent. The density functional theory used for carried out the theoretical conclusions (Ling et al., 2016). That were used for optimization of geometry and energy calculations. Vienna ab-initio simulation package used for performing these calculations (Lu et al., 2015; Zhang et al., 2014). These two result show that H of ribbons do an important features. Because of this is necessary to investigate systematically edge effect to PNRs with different chemical groups like OH, O, and COOH etc. in this investigation this demonstrate detailed analysis on the band structure and also density due to edge effect on APNRs as well as ZPNRs. By the using DFT the result comes out (Kohn & Sham, 1965). The energy which kinetic cutoff value this is basis set chosen as to be 500ev.

A distinctive Raman spectrum of phosphorene is obtainable. In agreement with former stories and the DFT designs, three Raman vigorous styles at occurrences 362, 440, and 466 cm^{-1} which can be observed and allocated to A_{1g}, B_{2g}, and A_{2g} regularities, correspondingly. (Ling et al., 2016). (Liu, Neal, Zhu, Luo, et al., 2014) by comparing with nil band gap graphene and also wide band gap boron nitride, that the BP retains reasonable direct bandgaps with the range of 0.6–1.5 eV, which is specific assessment be contingent on number of sheets. (Dai & Zeng, 2014; Guo, Lu, Wang, Wu, & Zeng, 2014).

Phosphorene has very interesting properties which are basically originated from its structure that have strong in plane covalent bond and weak van der Waals interlayer interactions (Bridgman, 1914; K. Novoselov et al., 2005). The interlayer distance of phosphorene varies between 2.37-2.40 Å which is best for mechanical exfoliation same as fabrication of graphene (Appalakondaiah, Vaitheeswaran, Lebegue, Christensen, & Svane, 2012; Churchill & Jarillo-Herrero, 2014). In the Brillouin Zone (BZ) close to the Fermi level, knowing about the phosphorene's attention gripping structural properties, its most amazing feature is high dispersion skill of anisotropic band. The desirable phosphorene which have high electrical conductivity and low thermal conductivity has boosted its thermoelectric performances. This is because of the electron transition in phosphorene which take place in armchair direction and causes low thermal conductivity (Bagheri, Chandrappa, & Hamid, 2013; Chekin, Bagheri, & Hamid, 2014; Kou, Chen, & Smith, 2015).

Later, transition metal dichalcogenides (TMDs) such as MoSe₂, MoS₂, and WSe₂ have inspired great extents of considerations owing to their layered arrangement equivalent to graphene with the extra advantage of an intrinsic band gap between ~0.4 to ~2.3 eV. As compared to TMDs, phosphorene carrier mobility has been agreed to be noticeably higher (Bagheri, Chekin, & Hamid, 2014; Qin et al., 2015). Due to its unique properties fabrication methods and new design phosphorene has wide range of application in various fields like field effect transistor (FET), gas sensors and batteries.

In 2014 positive fabrication of FET produced from phosphorene, there has been some significant growths that have established phosphorene new properties for diversity of areas such as gas sensors, electronic and transport properties. Also, phosphorene high charge carrier mobility at room temperature leads to sensibly fast operation. The properties are considerable in production of transistors with high current and power increases that are most

important features for designing the high frequency power amplifiers and high speed logic circuits. From the latest theoretical and investigational researches it has revealed that phosphorene is best for advanced battery applications having strong capacity of 2596 mAh/g and discharge potential range 0.4-1.2V. The high average voltage is expected of 2.9 V in phosphorene based Li-ion battery and outstanding electrical conductivity of phosphorene as an electrode suggest confident potential for its uses as rechargeable battery in many industrial fields (Kou et al., 2015). For gas sensing applications, phosphorene is considered as most appropriate single electron transistor (SET) (Er, Li, Naguib, Gogotsi, & Shenoy, 2014).

Computational Details

All the molecules have been optimized at the B3LYP and MPW1PW91 and PBE0 functional with 6-31G basis set. The absorption spectra have been calculated through time dependent DFT mean density functional theory adopting 6-31G basis set. The absorption spectra's calculation utilizing B3LYP and MPW1PW91 through adopting the basis set 6-31G. The energies at the level of density functional theory have been examined through the B3LYP and MPW1PW91 functional and basis set of 6-31G. All the calculations were carried out on Gaussian 09 packages of program. For the theoretical calculations this software is most popular and efficient (Marković et al., 2012). First of all, 3D structure of all molecules were designed on Gauss view 5.0 program (Dennington, Keith, & Millam, 2008).

Geometry optimization of design molecules phosphorene, polyaniline, and phosphorene with edge group COOH, phosphorene with edge group NH₂ and phosphorene with edge OH are done by DFT method. Firstly, all the designed molecules were calculated with DFT with different functions as B3LYP, CAM-B3LYP (Yanai, Tew, & Handy, 2004), MPW1PW91 (Adamo & Barone, 1998) for absorption spectra of designed molecules. MPW1PW91 is the best method for theoretical calculations for these molecules and therefore it was chosen for further optimization of molecules. For the theoretical calculations 6-31G (d,p) (Rassolov, Pople, Ratner, & Windus, 1998) basis set was used because it is time consuming, it gives reliable result for the geometry optimization with less cost (Zade, Zamoshchik, & Bendikov, 2009) TD-DFT with B3LYP, CAM-B3LYP and MPW1PW91 with basis set 6-31G (d,p) were used for absorption spectra of all these designed molecules. We got best absorption with function MPW1PW91/6-31G (d,p) of these molecules. So that we perform our further calculations by using MPW1PW91 and basis set 6-31G (d,p).

Designed Molecules

Molecule -1

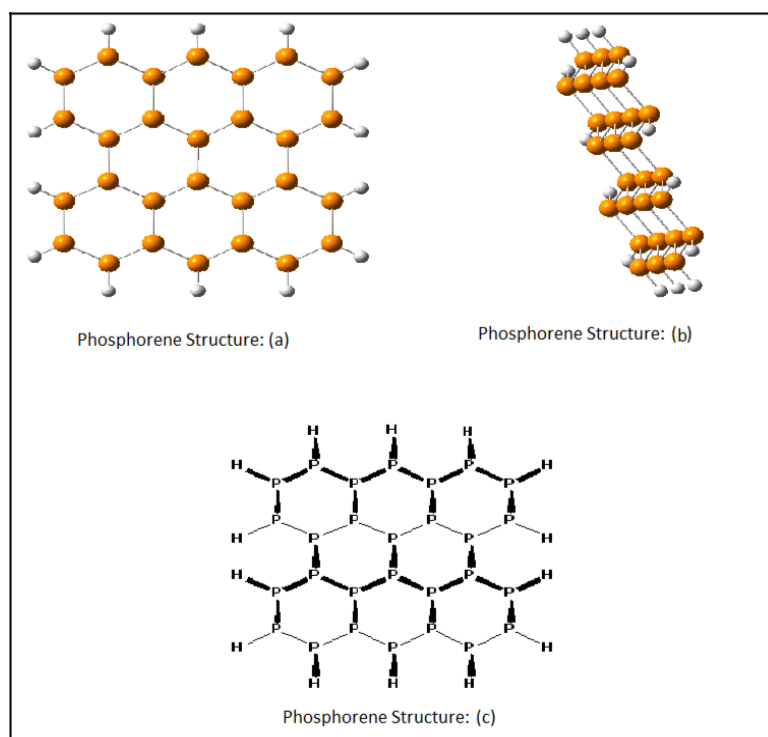


Figure 1 Phosphorene (a) Simple Gaussview (b) Zigzag Gaussview (c) Chemdraw ultra structure

Molecule -2

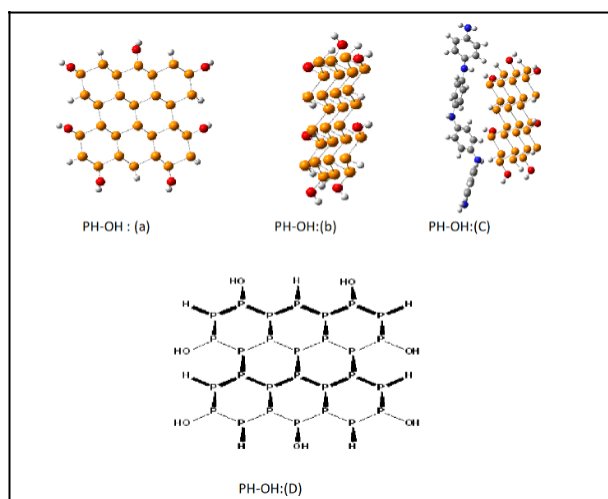


Figure 2 Phosphorene-OH structure: (a) simple gauss View (b) showing zigzag structure of gauss View (c). with –OH and polyanieline gauss view and structure (d) chem Draw Ultra structure

Molecule-3

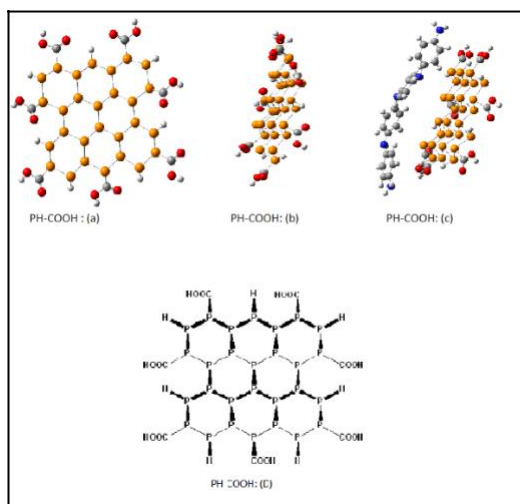


Figure 3 Phosphorene-COOH structure: (a) simple gauss View (b) zigzag structure of gauss View (c) with –COOH and polyanieline gauss view and structure (d) chem Draw Ultra structure

Molecule -4

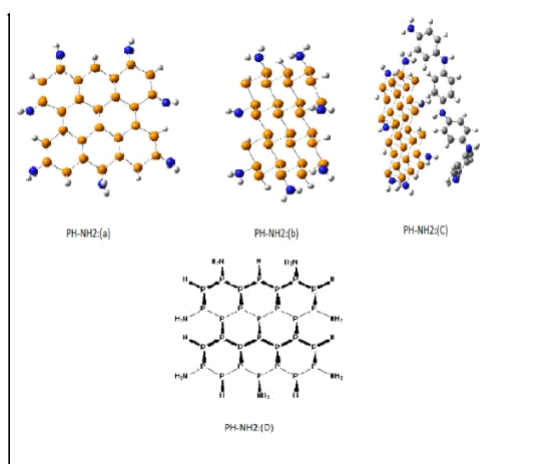


Figure 4 Phosphorene-NH2 structure: (a) simple gauss View (b) zigzag structure of gauss View (c). with –NH2 and polyanieline gauss view and structure (d) chem Draw Ultra structure

Results and discussions

Under the theory of DFT in computational chemistry there are performance of various functional groups with the designed molecule of phosphorene has been observed. The different functional groups and a polymer named as polyaniline examined by using the density functional theory (DFT) with the basis set B3LYP, CAM-B3LYP and MPW1PW91.

Optimization of molecular structure

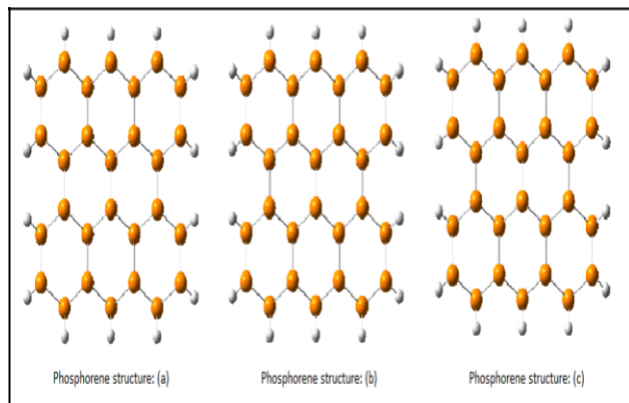


Figure 5 Optimized Phosphorene structures with B3LYP, CAM-B3LYP and MPW1PW91

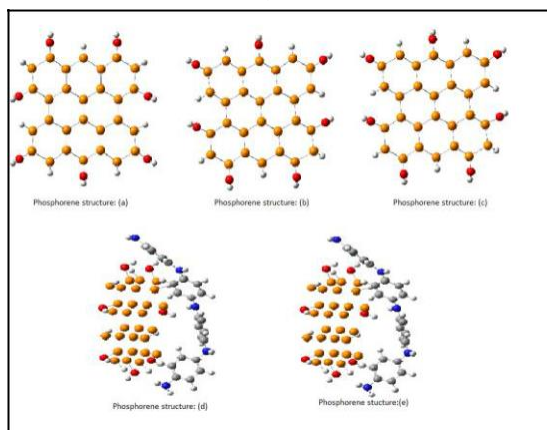


Figure 6 Phosphorene-OH structures from B3LYP, CAM-B3LYP and MPW1PW91 (a, b and c) Phosphorene-OH-PANI structures from B3LYP and MPW1PW91 (d and e)

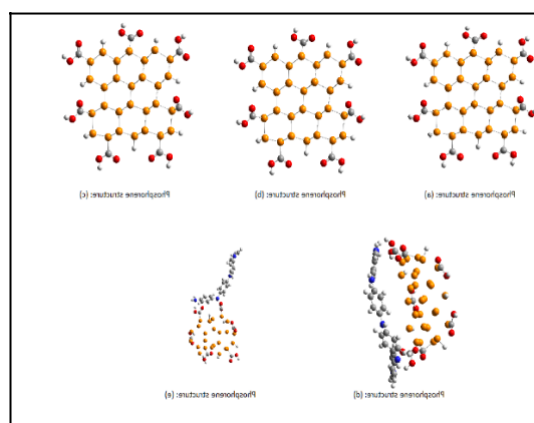


Figure 7 Phosphorene-COOH structures from B3LYP, CAM-B3LYP and MPW1PW91 (a, b and c) Phosphorene-COOH-PANI structures from MPW1PW91 and B3LYP (d and e)

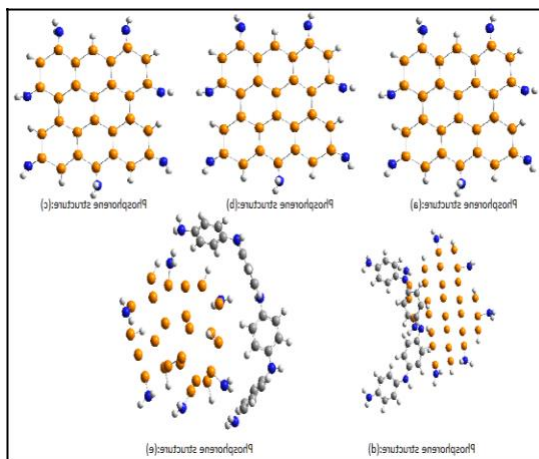


Figure 8 Phosphorene-NH₂ structures from B3LYP, CAM-B3LYP and MPW1PW91 (a, b and c). Phosphorene-NH₂-PANI structures from MPW1PW91 and B3LYP (d and e)

Optical properties

The frontier Molecular orbitals (FMOs)

The frontier molecular orbital (FMOs) that can be explained by the (HOMO) and (LUMO) the highest occupied molecular orbital and lowest unoccupied molecular orbital. The structures which are optimized with FMOs of designed systems under the basis sets of B3LYP, CAM-B3LYP and also MPW1PW91 shown in figures 4.1, 4.2, 4.3 and 4.4. One of the sophisticated thing in FMOs is the examination of molecules or compounds due to their exciting stuffs or applications.

The energy gap among E_{HOMO} and E_{LUMO} of the four molecules is started from 2.8275 eV to 3.484 eV phosphorene with functional groups –H, –OH, –COOH, and –NH₂ when the method used B3LYP and variation shown by phosphorene with polyaniline when the B3LYP method used. The molecule phosphorene with polyaniline and phosphorene with functional group –OH, –COOH, –NH₂ then the energy gap change from first molecules. Then the energy gap gradually increase from 1.619 eV to 2.741 eV from simple phosphorene with polyaniline and phosphorene with functional groups –OH, –COOH, –NH₂. In the method B3LYP the phosphorene with simple hydrogen band gap is 2.8275 eV and the wavelength about 365.3 nm and when the functional group attached with phosphorene then different wavelength are observed with different band gap such as –COOH, –OH, and –NH₂. The wavelength 508.62 nm 510.13nm and 380.35nm respectively. But the variation observed when phosphorene with functional group as well as polyaniline optimized.

Phosphorene with polyaniline when optimized then the band gap decrease to 1.6197 eV then the wavelength increased to 926.35 nm when B3LYP method used. This show that by decreasing band gap then wavelength increase. When the method changed to MPW1PW91 then also variations observed the simple phosphorene optimized then the band gap was 3.57eV and with the wavelength 343.84 nm the variation observed by using different functional groups with phosphorene by using MPW1PW91 method.

The results which are shown in the table 2 energy gap among E_{HOMO} and E_{LUMO} of all the phosphorene molecules between 2.166 eV to 4.231eV when the method MPW1PW91 used. When the band gap 3 eV or above the 3 eV then the wave length exhibited in the Ultra-Violet region. So the optoelectronic or optical properties observation displayed that when the band is small then the wavelength is high and if the band gap is large then wavelength shorter. When band gap is small then excitation will easy and more energy produce. The LUMO displayed antibonding and HOMO displayed the bonding orbital characters. So the pi-pi star transition always in lowest singlet state.so the energy gap among HOMO and LUMO is in order as:

Ph-pani-OH<Ph-pani-NH₂<Ph-pani-h<Ph-pani-COOH<Ph-h<Ph-COOH<Ph-OH<Ph-NH₂ having 2.166 eV, 2.238eV, 2.374eV, 2.629 eV, 3.577 eV, 4.131 eV, 4.167 eV, 4.231 eV respectively.

Table 1. Molecules with wavelengths, oscillatory strength, excitation energies:

Molecule	Function B3LYP ($\lambda_{\max}$ nm)	f	HOMO	LUMO	Difference (Ev)
Ph-H	365	0.034	-.22305	-.11915	2.827
Ph-OH	510	0.009	-.20215	-.12328	2.146
Ph-COOH	508	0.007	-.21619	-.13275	2.270
Ph-NH2	380	0.014	-.20414	-.07609	3.484
Ph-pani-H	926	0.001	-.14031	-.08079	1.619
Ph-pani-OH	553	0.002	-.15468	-.07972	2.039
Ph-pani-COOH	450	0.003	-.16758	-.08563	2.230
Ph-pani-NH2	463	0.002	-.17713	-.07638	2.741

Table 2. Molecules with wavelengths, oscillatory strength, excitation energies:

Molecule	Function MPW1PW91 ($\lambda_{\max}$ nm)	f	HOMO	LUMO	Difference (Ev)
Ph-H	343	0.0428	-.2317	-.1003	3.577
Ph-OH	371	0.0176	-.2315	-.7842	4.167
Ph-COOH	366	0.0246	-.2314	-.07962	4.131
Ph-NH2	344	0.0202	-.0.216	-.0.0614	4.231
Ph-pani-H	624	0.0023	-.1619	-.07466	2.374
Ph-pani-OH	542	0.0003	-.1594	-.07989	2.166
Ph-pani-COOH	502	.0004	-.1766	-.07999	2.629
Ph-pani-NH2	638	0.0055	-.1458	-.06350	2.238

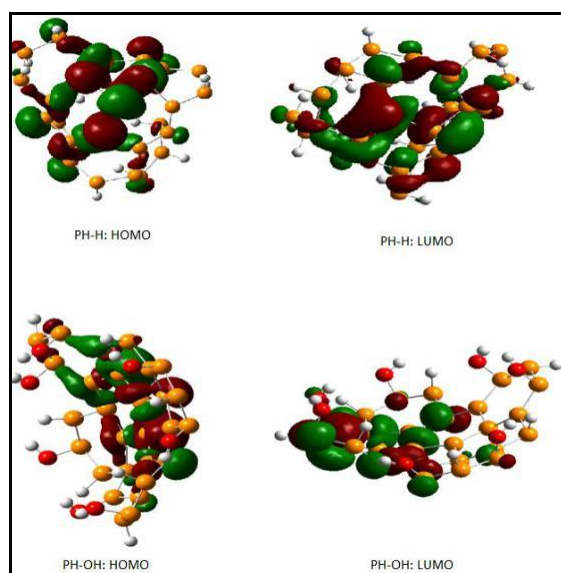


Figure 9 PH=Phosphorene, PH-OH= Phosphorene with –OH functional group HOMU and LUMO by the method MPW1PW91.

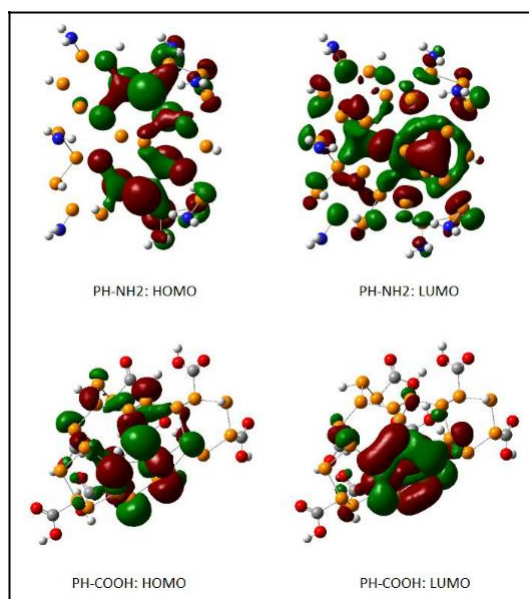


Figure 10 PH-NH₂= Phosphorene with functional group –NH₂, PH-COOH=Phosphorene with –COOH functional groups HOMO and LUMO when the method used MPW1PW91

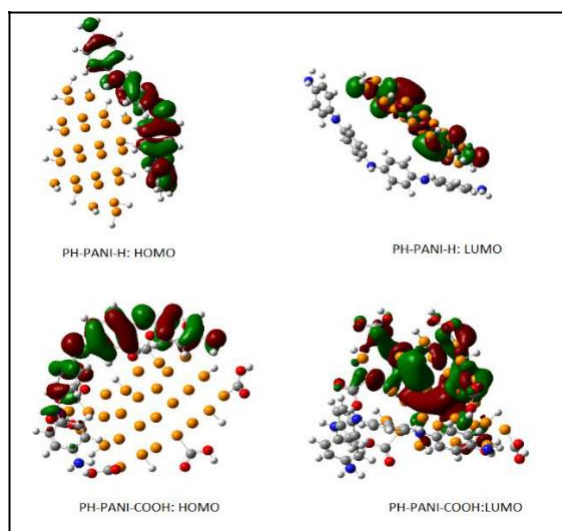


Figure 12 PH-PANI-H=Phosphorene with polyaniline, and PH-PANI-COOH=Phosphorene with functional group –COOH and Polyaniline HOMO and LUMO when the method used MPW1PW91.

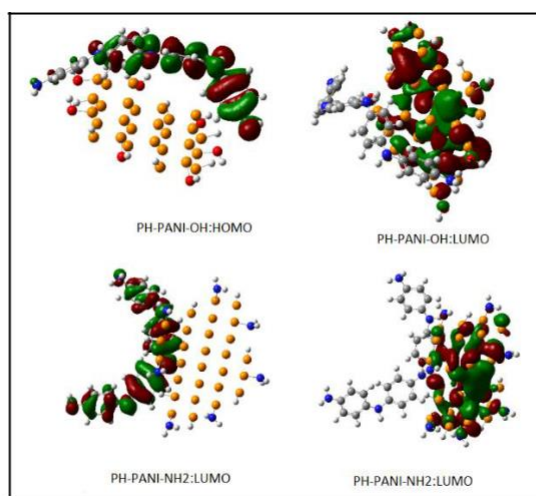


Figure 13 PH-PANI-OH=Phosphorene with functional group –OH and polyaniline, PH-PANI-COOH=Phosphorene with functional group –COOH and polyaniline HOMO and LUMO by MPW1PW91.

Dipole moment

Table 3 Dipole moments of every molecules are also calculated with the all chemical functional groups

Molecule	Dipole moment	Molecule	Dipole moment
PH-H	0.0006	PH-H-PANI	2.4038
PH-OH	6.4650	PH-OH-PANI	4.8428
PH-COOH	4.8222	PH-COOH-PANI	5.5670
PH-NH2	1.6522	PH-NH2-PANI	2.2735

Density of State

Density of state gives the electronic study of semiconductors. Density of state is the increment of energy per unit at the energy level. At the definite energy level the high density state presented that there is an extra energy level existing for occupation and no occupancy of energy level mean zero density state. In the density of state graphs there are four different colors red, green, black and blue the blue and green line display the HOMO while red line display the LUMO energy level respectively. So there is difference in those both line displaying the band gap (E_{gap}). Density state of phosphorene with different functional group with the method of MPW1PW91 are given above.

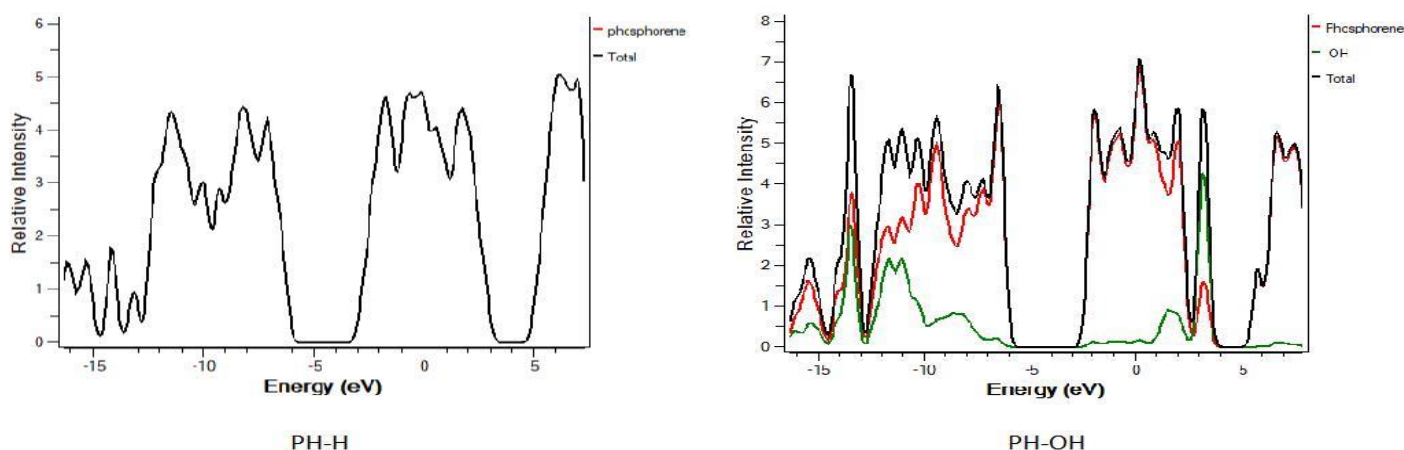


Figure 14 (a) and (b). Density of states (DOS) around HOMO and LUMO of phosphorene with functional groups and polyaniline

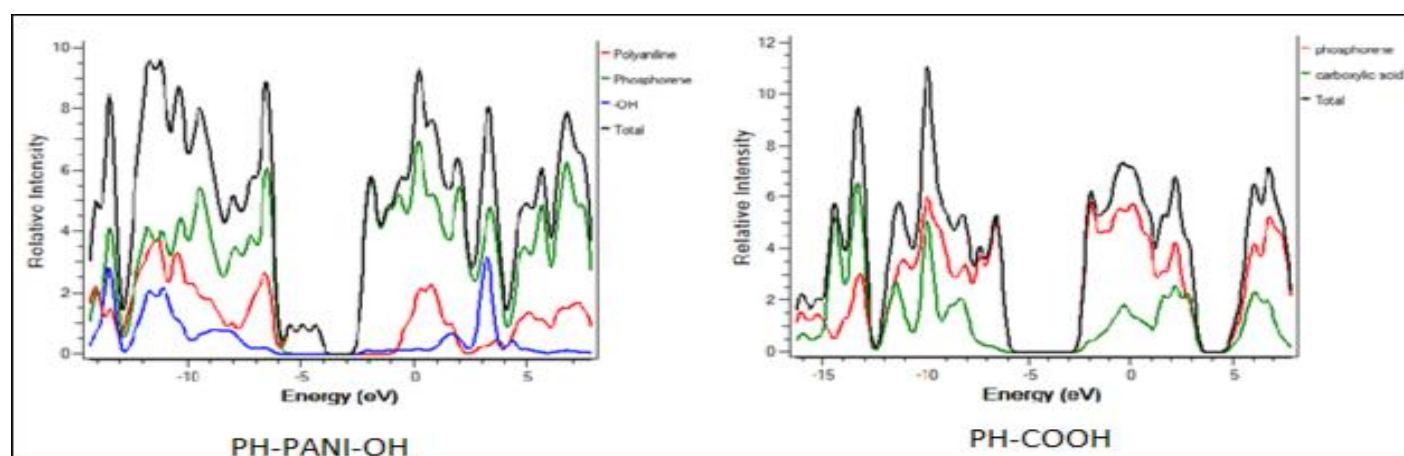


Figure 15 (a) PH=Phosphorene, PH-OH= Phosphorene with functional group –OH, PH-PANI-OH=Phosphorene with functional group –OH and Polyaniline and PH-COOH= Phosphorene with –COOH.

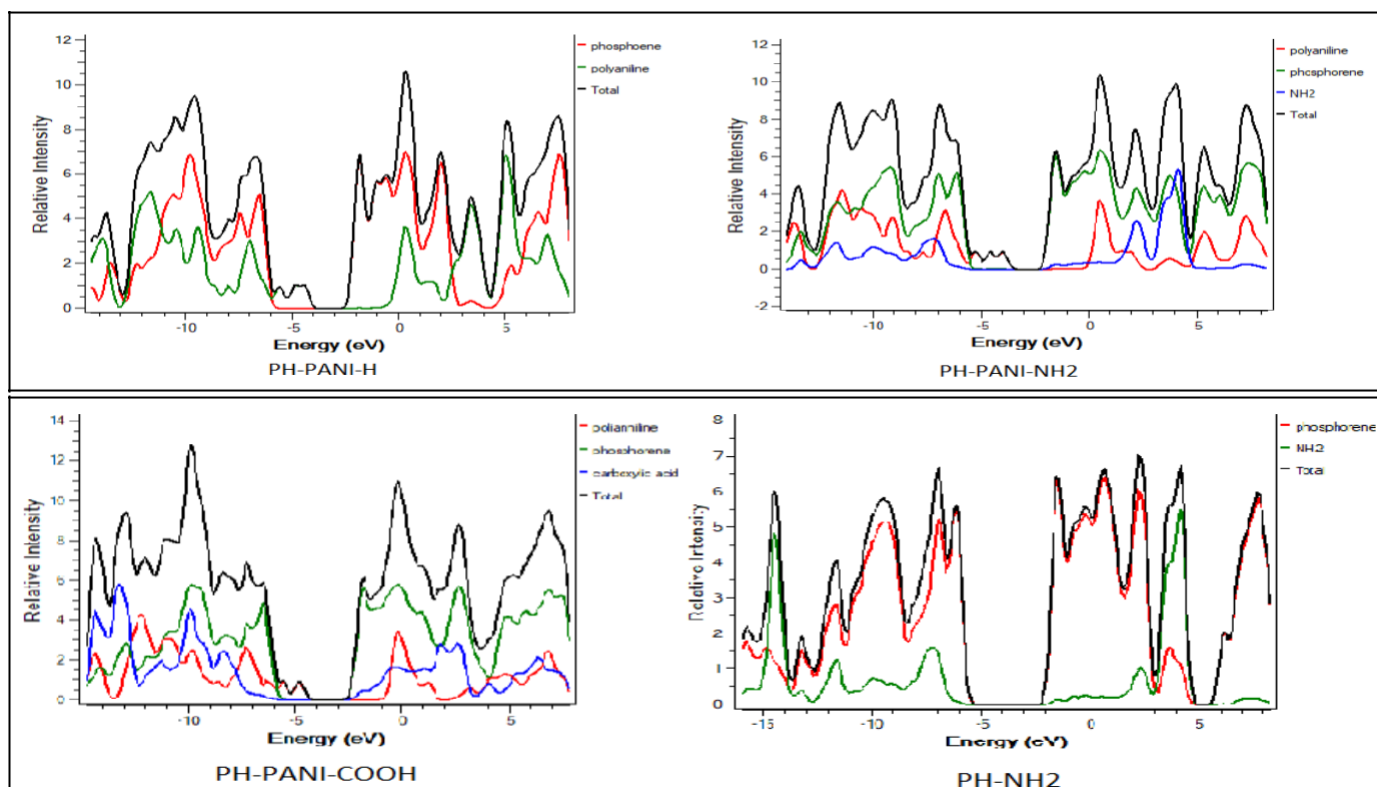


Figure 15 (b) PH-PANI-H=Phosphorene with polyaniline and –H and PH-PANI-NH2= Phosphorene with functional group –NH2 and polyaniline, PH-PANI-COOH=Phosphorene with functional group –COOH and polyaniline and PH-NH2= Phosphorene with –NH2 functional group.

Absorption spectra's

The absorption spectra's are calculated by using the TD-DFT. The absorptions spectra's of phosphorene with different functional groups and polyaniline are resulted as by using the two different methods B3LYP and MPW1PW91. The absorption spectra's display that when the band gap is shorter than the longer wavelength is obtained. This results display that at small band gap then the excitation will be easy and that resulted the longer wavelength energy production is more.

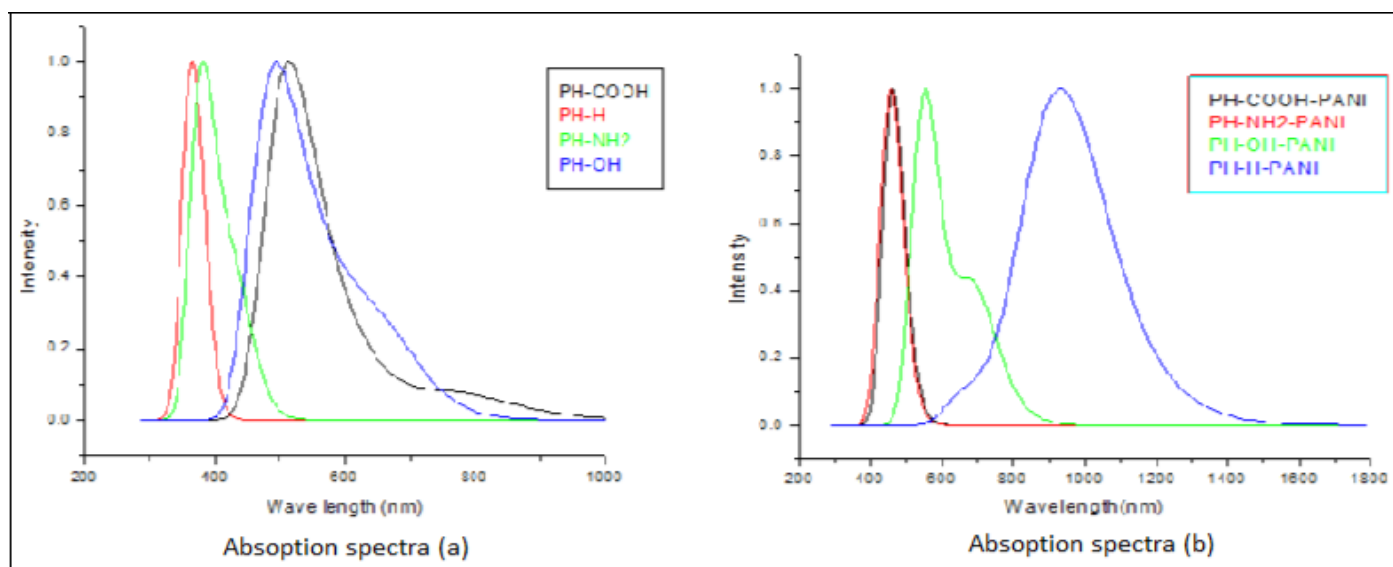


Figure 16 The absorption spectra's (a and b) are resulted when the method used B3LYP.

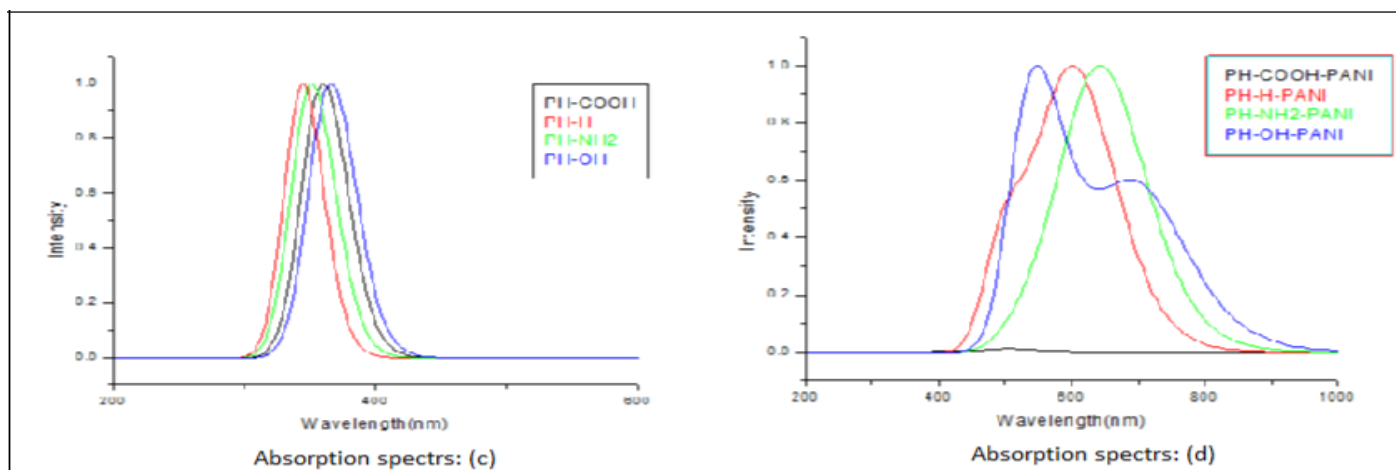


Figure 17: The absorption spectra's (c and d) are resulted when the method used MPW1PW91.

Conclusions

Under the method of DFT in computational chemistry there are presentation of different chemical functional groups with the designed molecule of phosphorene has been examined. The various chemical functional groups and a polymer named as polyaniline examined by using the density functional theory (DFT) with the basis set B3LYP, CAM-B3LYP and MPW1PW91. The best method MPW1PW91 selected for further results. The results are discussed as on the basis of wave lengths and band gap. These two properties give more information about the optoelectronic assets. The optoelectronic properties concern to the band gap and excitation of electrons. In this effort we observed that when by using the method MPW1PW91 in the Phosphorene molecule then the wave length and band gap gives variation by using different chemical functional groups. Especially when the phosphorene with functional groups – OH, -COOH and -NH₂ with polyaniline resulted the less band gap and longer wavelength. This property show that the excitation is easy and wavelength in the visible range so that gives the more energy production. When the band gap 3 eV or above the 3 eV then the wave length exhibited in the Ultra-Violet region. So the optoelectronic or optical properties observation displayed that when the band is small then the wavelength is high and if the band gap is large then wavelength shorter. Another property discussed above is that there is charge transfer between Phosphorene molecule and the polyaniline polymer because the electron density change between molecule and polymer respectively with HOMO and LUMO level which show the charge transfer mechanism.

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