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A DFT Study of Optoelectronic Properties and Electronic Structure of Edge-Modified Phosphorene Quantum Dots Interacting with Polyaniline

Faheem Abbas[1], Muhammad Shoaib[2], Muhammad Ishaq[3], Muhammad Rais Aslam[4], Muhammad Umar[5], Muhammad Irfan Haider[6], Iqra Farooq[7]
[1, 2, 3, 4, 7]Department of chemistry, University of Agriculture Faisalabad, 38000, Faisalabad Pakistan
[5, 6]Department of chemistry, Government College University, Faisalabad Pakistan

Abstract: There are recent results of experiments on the edge-functionalization of phosphorene Quantum dots (PQDs) also with conductive polymer for the production of energy. Now we have examined that influence of Phosphorene Quantum Dots in addition to Polyaniline found significant modification in optical properties as well structural properties. In this effort we demonstrate a mixed methods for the determination of optical properties as well as physical properties. Results shows that the Phosphorene Quantum Dots (PQDs) favor the edge modification with PANI/PQDs interaction that helping a very stimulating electronic properties. Mainly when –OH and –COOH functional groups are existing at the edge of Phosphorene Quantum Dots (PQDs) a very decent electronic hole separation in duration of photon excitation is found. That establish its potential for optoelectronic uses. Single-electron transistors, solar cells, LEDs, lasers, single-photon sources, second-harmonic generation, quantum computing, and medical imaging are possible applications of quantum dots. Their small size allows the suspension of some QDs in solution, which may result in use in inkjet printing and spin-coating.

I. INTRODUCTION

In 1669 the brandt was discovered first time phosphorus the 11th abundant element of earth crust [1-4]. Phosphorus is highly reactive with oxygen it is not found in the elemental form in nature comparing it with the other group elements like carbon as well as Sulphur [5, 6]. Naturally phosphorus is in the form of phosphate which importance overcome frontier of inorganic chemistry. Phosphate as well as its derivatives central in industrial sectors like fertilizers and cleaners etc. it is also a point out that its importance in living beings like energy change such as ATP in the RNA and DNA and other process also growth and teeth formation and bone also [7]. In the world the technique which is used is temperature treatment to obtain the phosphorus in elemental form from Mineral phosphates this treatment is done with reducing agents like carbon coke. White phosphorus is obtain as final product which is P4 tetrahedral structure [8]. And having lone pair on the every phosphorus atoms.

That white phosphorus is precursor of organo phosphorus when treatment with chlorine which is molecular form and the substrate used to introduce the substituents at phosphorus center [9]. The red phosphorus allotrope is obtain when white phosphorus is heated. That show 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[10]. The polymerization degree of black phosphorus shared with red. This show the orderly the layered structures with the distance of interlayers is 3.11 A° [11].

It marginally investigate after this discovery for many decades. The blooming attention were assisted by chemist and physists in 2015which is gradually increased in in these years. The mainly this due to physical and electrical may be electronic features exfoliated black phosphorus monolayer also called phosphorene.[12]. Phosphorene (BP) a layered material emerged as favorable 2D material because of its direct band gap, behavior of ambipolar, also having mechanical flexibility with greater carrier mobility[13, 14]. The single and few layered phosphorene synthesis by adopting method of exfoliation recently demonstrated. The layered structure of phosphorene inside each phosphorus atom is bonded with three other phosphorus atom forming to the structure like honeycomb similarly to the structure of graphene.

But graphene has zero band gap and phosphorene having band gap 0.3eV in bulk material which increase up to 1.0-1.5 eV when monolayer is isolated[15, 16]. Due to band gap and also the electric behavior ambipolar phosphorene attractive for optoelectronic devices which are operating in visible also in the near infrared regions[17]. And the transistor based upon phosphorene demonstrate high on/off ratio ($>10^5$) and also having great carrier mobility (300-1000 cm2 V-1 s-1)[12, 18]. By the connection of phosphorene with MOS_2 possible to engineer the junction (p-n) of 2D for solar harvesting as well as photo detection[19].

Another emerging field where phosphorene finds its assets as in energy storage, especially rechargeable batteries. There are currently popular energy devices are li-ion batteries having large applications as well as long term but have some critical concerns due to limited lithium and high price[20]. So Na-ion batteries in which phosphorene used as anode material receive more attention recently due to low-cost, large-scale application[21, 22].The phosphorene structure non-flat and anisotropic leads to specific orientation-dependent thermoelectric as well as optoelectronic assets[23]. Which newly attract the attention of researcher due to their specific properties like electric am bipolar, band gap, carrier mobility in the area of optoelectronic devices. Because of the demand of devices which are more reliable due to their performance excessive deal tries made near the material which are layered with extraordinary properties like carrier mobility and band gap. Between the allotrope of phosphorus[12] the BP which is most stable one 2D material which have layered structure and weak Vander Waal forces [16]. Our research group systematically examined the effect of two different groups and studied the electronic and optical properties through FMOs study.

II. COMPUTATIONAL DETAILS

All calculations regarding to optoelectronic properties are performed on Density functional Theory [24]. Our task is to calculate exactly first principle calculations concerning an important number of atoms. Our task is limited by the computational cost. In order to make the sensible starting DFT using the software Guassian09 [25]. For the best method we optimized our designed structures PH-X where X=H, COOH, OH and NH_2 and polyaniline with DFT functional B3LYP[26] and MPW1PW91 [27] with basis set 6-31G (d,p) level of theory to evaluate the optoelectronic properties of our designed structures. After observing the experimental data (absorption values) of B3LYP and MPW1PW91. The maximum absorption values of MPW1PW91 are gradually increases with sequence. MPW1PW91 with basis set of 6-31G (d,p) chosen the best method for further procedure Then finally we continue the time dependent density functional theory TD-DFT using the similar situation at MPW1PW91 with 6-31G (d,p) basis set for examination of optical assets. So, all the calculations carried out with functional MPW1PW91and basis set 6-31G (d,p) level of theory. The density of state (DOS) calculations are also achieved at MPW1PW91/6-31G (d,p) level of theory. PyMOlyze software [28] was used for DOS spectra and UV/Vis spectra of molecules are also obtained to investigate optoelectronic properties. Origin 6.0 program is used to obtain the absorption spectra[29].

III. RESULTS AND DISCUSSIONS

The above mention, all the different functional B3LYP and MPW1PW91 the method MPW1PW91 with basis set 6-31G (d,p) was chosen for the further calculations. UV/Vis spectra of absorption λ_{max} of Phosphorene with polyaniline at B3LYP, MPW1PW91 is 926nm, and 624nm respectively.

A. Frontier Molecular orbitals (FMO's)

The molecular structure of phosphorene with different chemical functional groups are illustrated in Figure 1, and optimized geometry of all structures with different functional group at MPW1Pw91 are shown in Figure 2. The frontier molecular orbital (FMOs) that can be explained by the (HOMO) highest occupied molecular orbital and (LUMO) the lowest unoccupied molecular orbital. The word energy gap refer to the energy difference among the top of valence and the bottom of conduction band. The modern surge of movements in the wide band gap materials risen form the necessity for the devices which are electronic proficient of operation at great power levels, temperature, caustic environments and distinctly a requirement for optical materials particularly emitters, which are active in blue and ultraviolet regions. For the description of optical as well as electronic assets the examination of distribution design of FMOs are actually valuable. The optimized geometry of all molecules with functional MPW1PW91 are illustrated in Figure 3. The structures which are optimized are used to approve the planer structures of fragments or molecules where the capability of delocalization of electrons within the organization or arrangement of molecule through the conjugation which increase the carrier movement or mobility. 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 are started from 2.82 eV to 3.48 eV when phosphorene with functional groups –H, –OH, -COOH, and –NH2 variation shown by phosphorene with polyaniline when the method used B3LYP. When the molecule phosphorene with functional group –OH, -COOH, -NH2 as well as polyaniline then the energy gap gradually increase from 1.619 eV to 2.741 eV. 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.

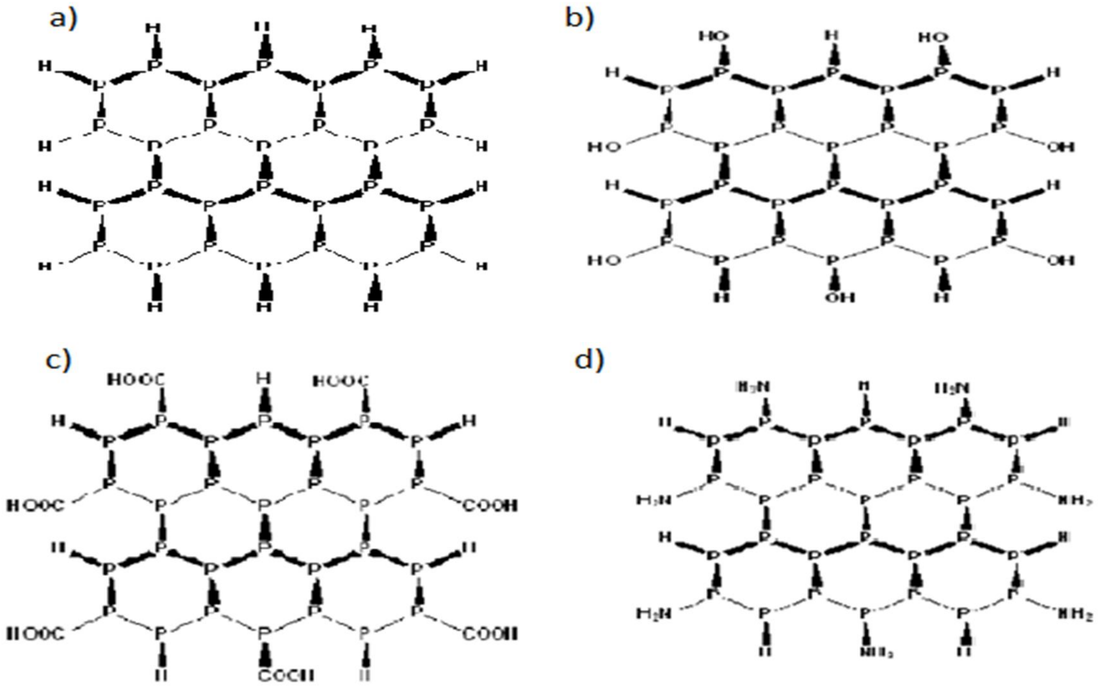


Figure 1. Molecular structures of phosphorene with different chemical functional groups –H, OH, COOH and NH_2 in structure a, b, c and d respectively.

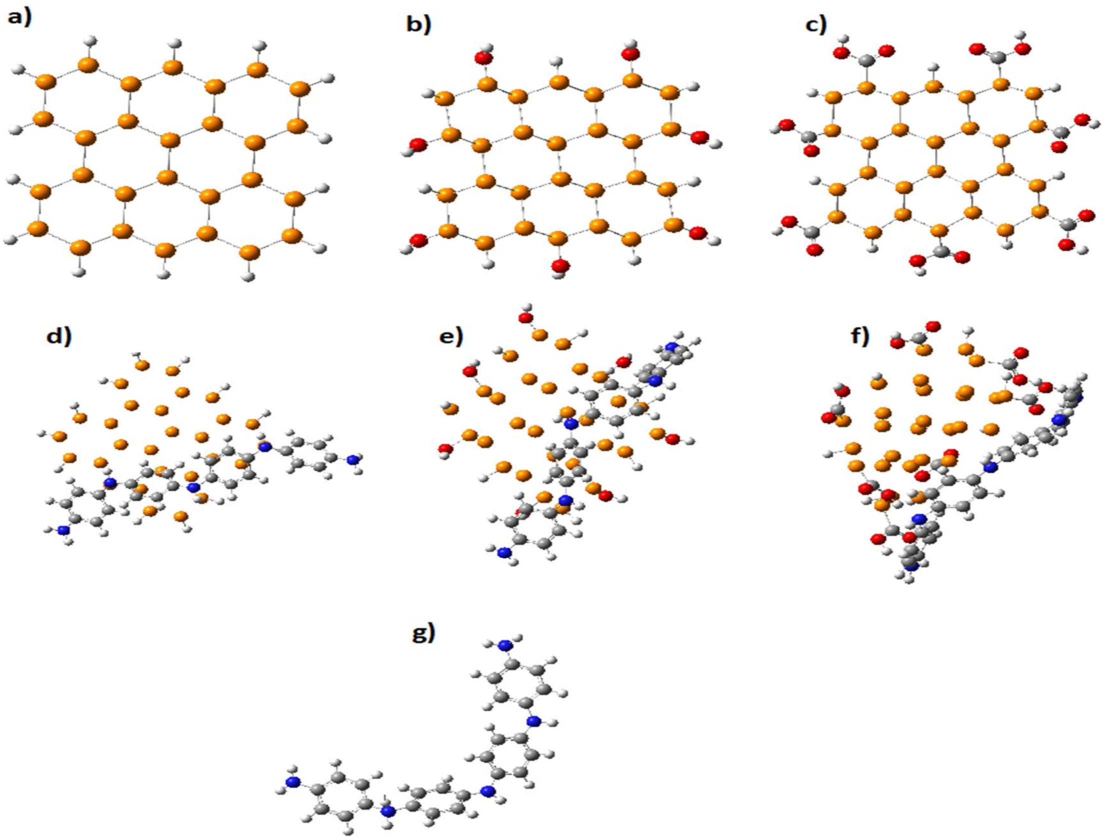


Figure 2. Optimized Structure and geometry for PH−X with (a) X = H, (b) X = OH, (c) X = COOH, (d) X = H and PANI, (e) X=OH, PANI (f) X= COOH and PANI and (g) = PANI.

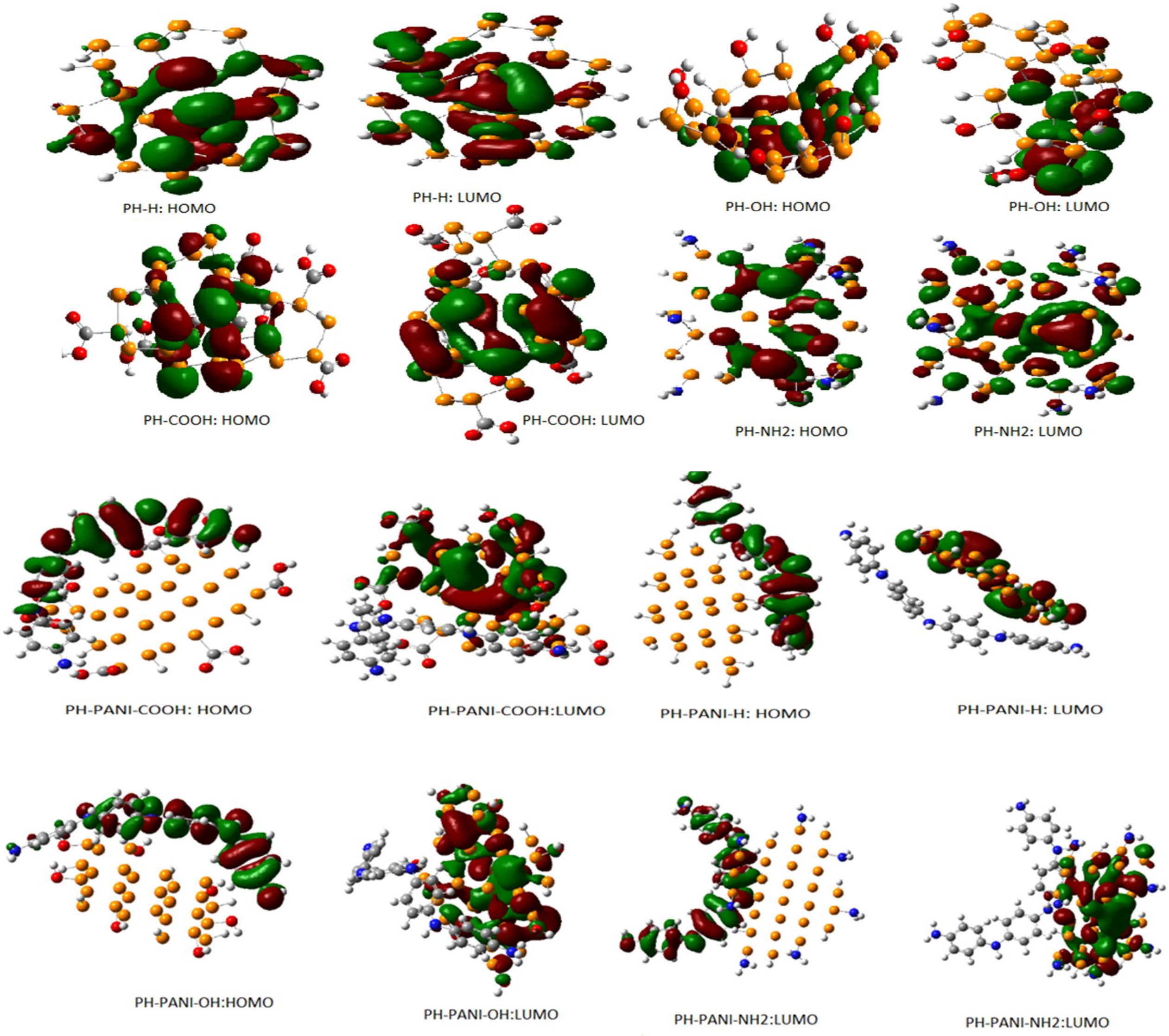


Figure 3. FMO of Phosphorene with different chemical functional groups and polyaniline at MPW1PW91 6-31 G (d,p) level of theory.

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

Molecule	Function B3LYP (λ_{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
Ph=phosphorene, *f*=oscillatory strength					

When the method changed to MPW1PW91 then variations also obtained. The simple phosphorene optimized then the band gap was 3.57 eV and with the wavelength 343.84 nm the variation observed by using different functional groups with phosphorene with MPW1PW91 method.

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

Molecule	Function MPW1PW91 (λ_{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

The results 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 properties observation displayed that when the band gap 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 because of DE stability 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. Distribution pattern around HOMO and LUMO are illustrated the charge transfer properties in molecule of phosphorene with polyaniline. When there is no polymer with in the molecule of phosphorene then the electron density equally distributed at the molecule of phosphorene with all functional groups PH-H, PH-COOH, PH-OH and PH-NH2 respectively result shown below But different results obtained when the phosphorene is optimized with polymer polyaniline then electron density change between HOMO and LUMO. Because the charge transfer occur between phosphorene and polymer (polyaniline) as shown through HOMO and LUMO in Figure 3.

IV. DIPOLE MOMENT

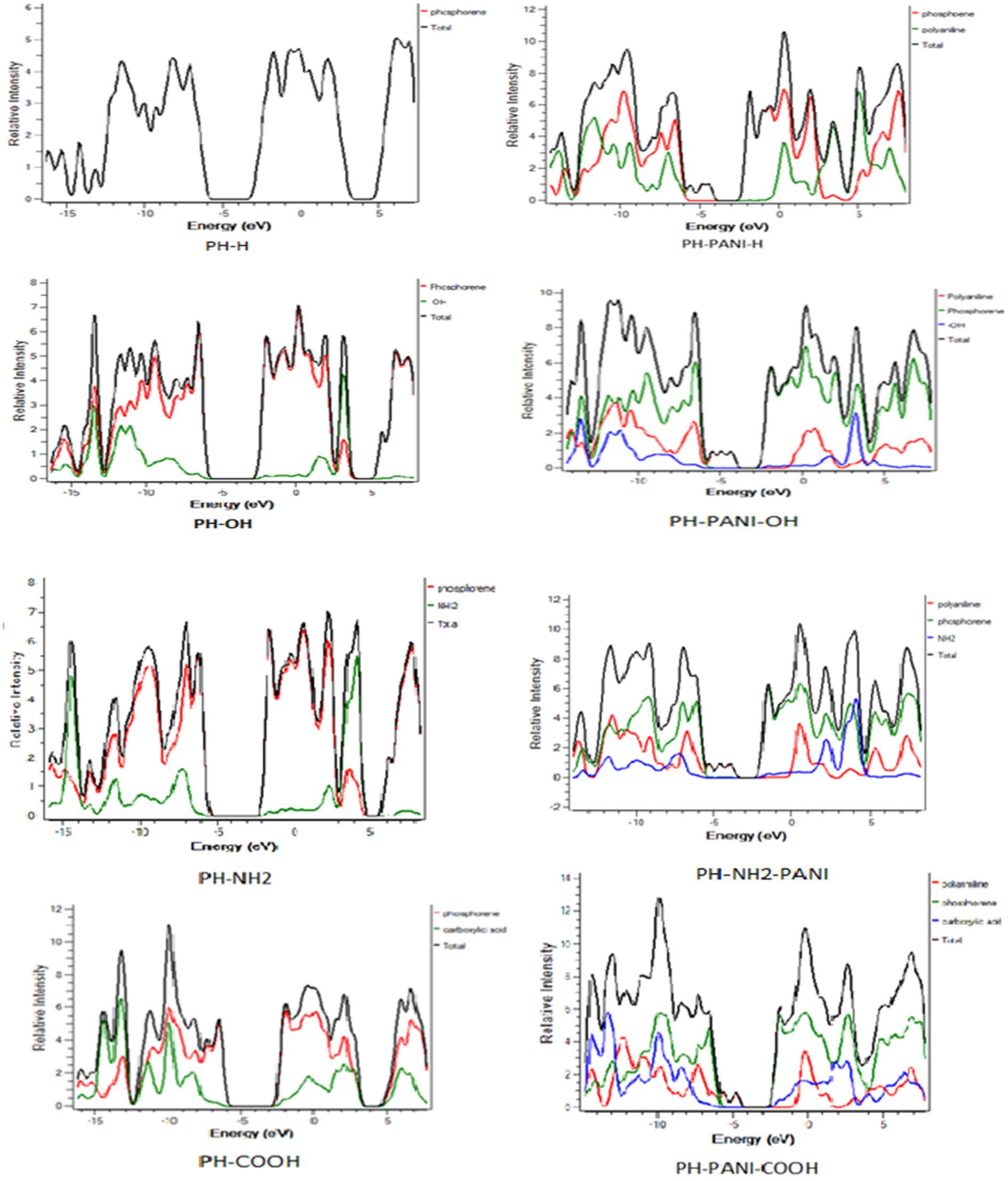
Dipole moments of every phosphorene molecules with same selected functional MPW1PW91/6-31G (d,p) basis set are calculated with the all chemical functional groups. The dipole moments have unlimited effect on fabrication procedure of optoelectronic devices which is connected to solubility's in solvents of organic. Solubility and Dipole moment are correlated to one another. The greater dipole moment value means the greater solubility in organic solvent and higher charge transfer rate[30]. The dipole moment of designed phosphorene molecules with different chemical functional groups are increasing in order PH-H<PH-NH2<PH-NH2-PANI<PH-H-PANI<PH-COOH<PH-OH-PANI<PH-COOH-PANI<PH-OH are shown in Table 3.

Table 3. The designed molecules with its Dipole moment.

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

V. DENSITY OF STATE (DOS)

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 of state of phosphorene with different chemical functional groups and polyaniline with the method of MPW1PW91 are given in Figure 4.



PH-H

PH-PANI-H

PH-OH

PH-PANI-OH

PH-NH2

PH-NH2-PANI

PH-COOH

PH-PANI-COOH

Figure 4. Density of states (DOS) around HOMOs and LUMO of Phosphorene with chemical functional groups and polymer polyaniline at MPW1PW91/6-31G (d,p) level of theory.

VI. OPTICAL PROPERTIES

To obtaiend the optical properties of phosphorene with edge chemical functional groups and polyaniline we performed TD-DFT calculations at MPW1PW91/6-31G(d,p) level of theory it showed the excitation transition of first 10 singlet to singlet states but the first excitation state we only consider due to the most significant with PH-H-PANI, PH-COOH-PANI, PH-NH_2-PANI and PH-OH-PANI structures with maximum absorption value (λ_{max}), Major contribution (electronic transition contribution, ETC %) and oscillator strength (f) as shown in Table 4. The ranges of absorption spectra from 343nm to 638nm.

Tabele 4. Wavelength (nm), oscillator strength(f), ETC % and E_{ev} for phosphorene with different chemical functional groups and polyaniline.

Molecules	Wavelength (λ_{max} nm)	E_{ev}	Oscialltion strength (f)	Major contribution (ETC %)
PH-H	343	3.577	0.0428	H-1->L+0(+80%)
PH-OH	371	4.167	0.0176	H-0->L+1(+68%)
PH-COOH	366	4.131	0.0246	H-0->L+0(+56%)
PH-NH2	344	4.231	0.0202	H-0->L+0(+82%)
PH-PANI-H	624	2.374	0.0023	H-0->L+0(+97%)
PH-PANI-OH	542	2.166	0.0003	H-0->L+0(+92%)
PH-PANI-COOH	502	2.629	0.0004	H-0->L+0(+99%)
PH-PANI-NH2	638	2.238	0.0055	H-0->L+0(+97%)

The absoroption band of all Phosphorene molecules with chemical functional groups are in the range from 343 nm to 638 nm. The λ_{max} of all molecule are shown in Table 4. Among all the molecule the λ_{max} increases from simple phosphorene to phosphorene with polymer polyanniline. The λ_{max} are in order PH-H<PH-NH2<PH-COOH<PH-OH<PH-PANI-COOH<PH-PANI-OH<PH-PANI-H<PH-PANI-NH2.

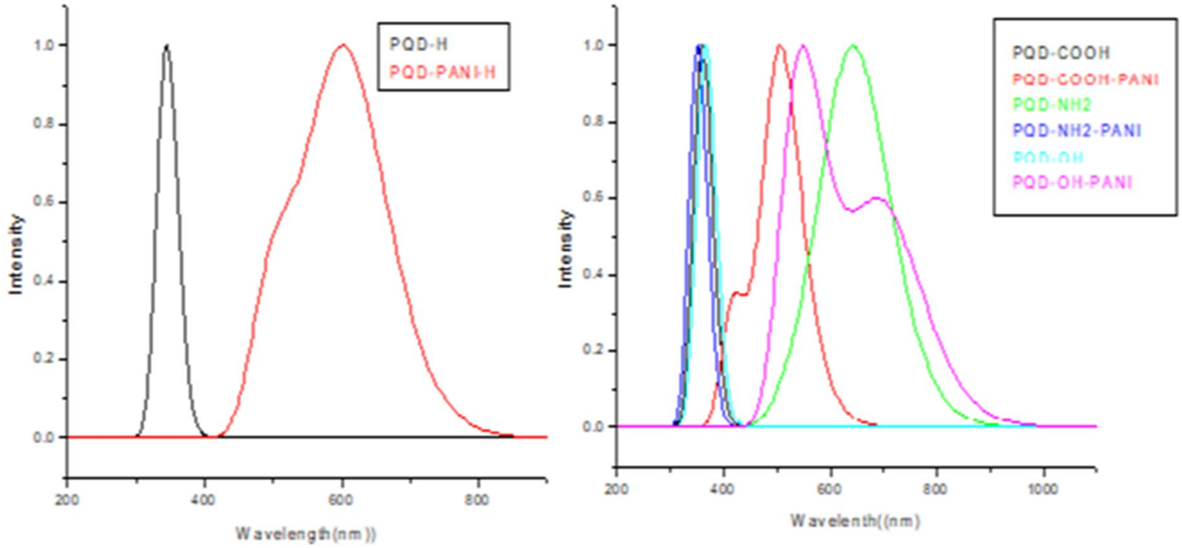


Figure 5. Simulated absorption spectras for PQD-H, GQD–PANI-H, and PGQD–COOH, PQD-COOH-PANI, PQD-NH2, PQD-NH2-PANI, PQD-OH and PQD-OH-PANI respectively at TD-MPW1PW91/6-31G(d,p) level of theory.

From the above explianation it can peridicted that among all the phosphorene with all chemical functional groups with polynniline show the best optical properties especially when the phosphorene with polynniline and phosphorene-NH2 polyaniline show the absorption high from others. The simulated absorption spectra are shown in Figure 5.

VII. CONCLUSIONS

By using DFT Method we have presented a mixed procedure followed by TD-DFT designs. We presented that the interaction of electrons between polymer polyanniline(PANI) and PQDs is improved when oxidizing groups like (–OH,-COOH) and the chemical functional group –NH2 are incorporated in the PQD, which further presents structural asymmetries, which is very applicable for the properties which are related to optical. In specifically, the presence of polyaniline polymer with the chemical functional groups at the edges of the PQD−OH-PANI and PQD−COOH-PANI and PQD-NH_2-PANI decreases the electronic topography symmetry, favoring the charge departure upon an optical excitation, thus founding a very promising system for optical uses in general and organic solar cells in particular.

VIII. ACKNOWLEDGEMENT

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A. Conflict of Interest

There are no conflict of interest.

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