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ORIGINAL ARTICLE

# DFT theoretical investigations of $\pi$ -conjugated molecules based on thienopyrazine and different acceptor moieties for organic photovoltaic cells



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## KEYWORDS

$\pi$ -Conjugated molecules;  
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DFT;  
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Electronic properties;  
 $V_{oc}$  (open circuit voltage)

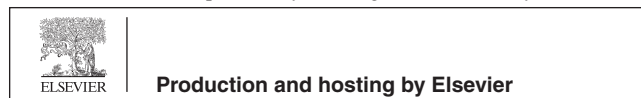
**Abstract** In this work, theoretical study by using the DFT method on eleven conjugated compounds based on thienopyrazine is reported. Different electron side groups were introduced to investigate their effects on the electronic structure; The HOMO, LUMO and Gap energy of these compounds have been calculated and reported in this paper. A systematic theoretical study of such compound has not been reported as we know. Thus, our aim is first, to explore their electronic and spectroscopic properties on the basis of the DFT quantum chemical calculations. Second, we are interested to elucidate the parameters that influence the photovoltaic efficiency toward better understanding of the structure–property relationships. The study of structural, electronic and optical properties for these compounds could help to design more efficient functional photovoltaic organic materials.

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## 1. Introduction

The research of new material based on  $\pi$ -conjugated molecules has become one of the most interesting topics in the fields of chemistry, physics and material science. Due to their specific

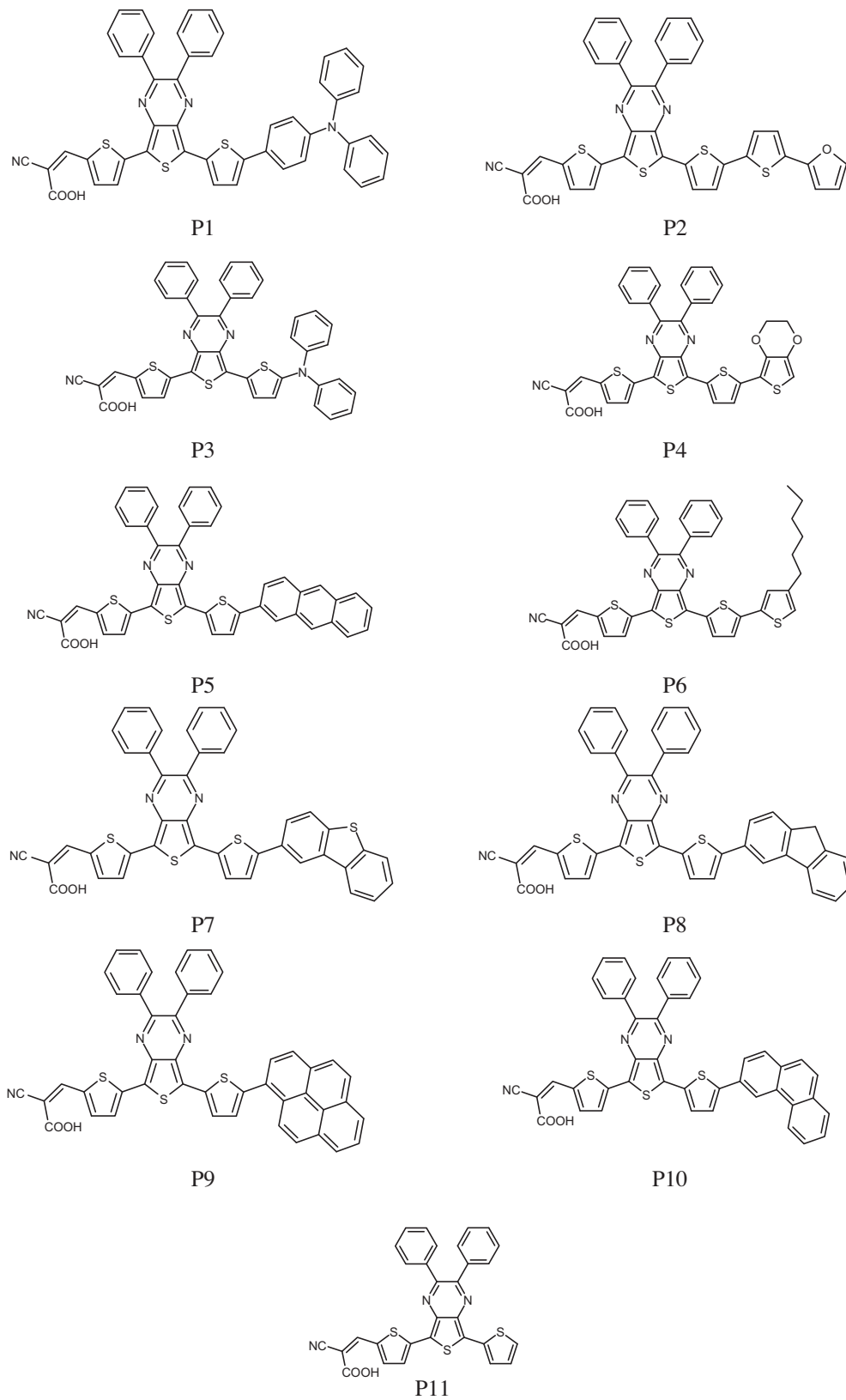
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properties, these compounds become the most promising materials for the optoelectronic device technology (Nalwa, 1997; Nguyen and Potje-Kamloth, 1999; Li et al., 2002), such

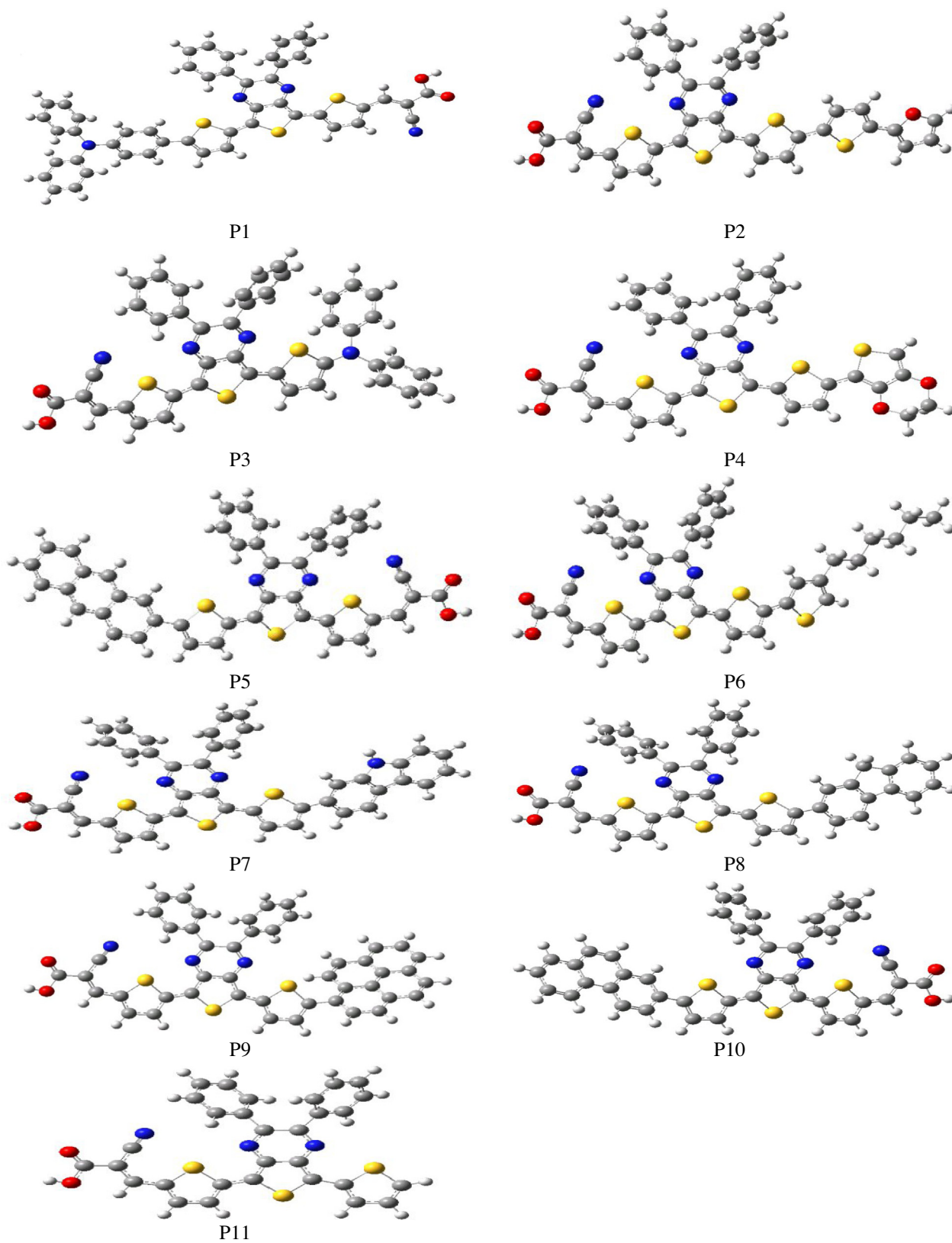
as LEDs (Gill et al., 1994), Transistors (TFTs) (Garnier et al., 1990) and solar cells (Wang et al., 2000; Chen et al., 2009a). Many researchers have been interested in synthesizing



**Figure 1** Chemical structure of studied compounds  $P_i$  ( $i = 1-11$ ).

short-chain compounds based on conjugated molecules because they are not amorphous and can be synthesized as well defined structures (Velusamy et al., 2005; Müllen and Wegner,

1998; Cornil et al., 1998; Li et al., 2009a,b, 2010). On the other hand since the discovery of the ultra fast and ultra efficient photo induced electron transfer between  $\pi$ -conjugated systems

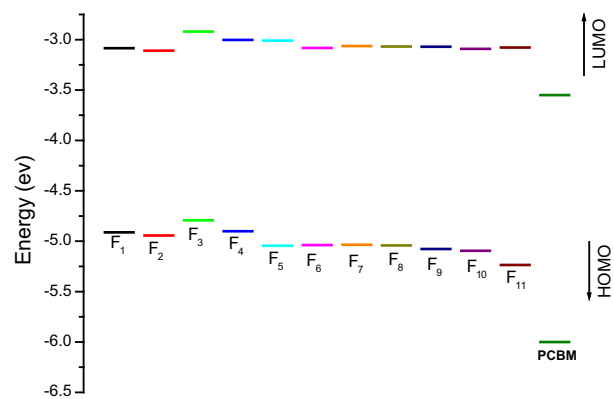


**Figure 2** Optimized geometries obtained by B3LYP/6-31G (d, p) of the studied molecules.

and fullerene derivatives (Shaheen et al., 2001; Padinger et al., 2003) considerable interest for hetero-junction solar cells based on interpenetrating networks of conjugated systems and C60 derivatives has been generated (He et al., 2010). (Roquet et al., 2006) reported the relationships between the nature of acceptor groups in the molecule and the photovoltaic performance. The results show that the introduction of electron-acceptor groups in the donor structure induces an extension of the photo-response in the visible spectral region, an increase of the maximum external quantum efficiency and an increase of the open circuit voltage under white light illumination. The use of low band gap materials is a viable method for better harvesting of the solar spectrum and increasing its efficiency (Chen et al., 2009b). The control of this parameter of these materials is a research issue of ongoing interest. This band gap engineering gives this material its desired electrical and optical properties, reduction of band gap to approximately zero is expected to give an intrinsically conducting material. The most efficient strategy has been applied to design molecules which alternate donor-acceptor repeating units that are expected to have small gaps (Cravino and Sariciftci, 2002; Roquet et al., 2006).

In parallel with new experimental results on these new materials, theoretical investigations have indeed begun to constitute an important source of valuable information which supplements the experimental studies, thereby contributing to the rationalization of the properties of known materials and the prediction of those yet unknown (Bouzakraoui et al., 2005, 2006; Zgou et al., 2008; Bouzzine et al., 2008; Mondal et al., 2010).

In this context and in order to guide the synthesis of novel materials with low band gaps, quantum-chemical methods have been increasingly applied to predict the band gap of conjugated systems. We note that theoretical knowledge of the HOMO and LUMO energy levels of the components is basic in studying organic solar cells. So, we can save time and money in choosing the adequate organic materials to optimize photovoltaic device properties. The HOMO and LUMO energy levels of the donor and acceptor components are very important factors to determine whether an effective charge transfer will happen between donor and acceptor. The offset of band edges



**Figure 3** Sketch of B3LYP/6-31G (d, p) calculated energies of the HOMO, LUMO level of studied molecules.

of HOMO and LOMO levels will prove responsible for the improvement of all photovoltaic properties of the organic solar cells.

Recently, the compounds with D- $\pi$ -A structure are described and studied by different authors who have shown the importance of these materials in use as a solar cell. (Tian et al., 2010, Han, 2011; Pasunooti, 2011; Bundgaard and Krebs, 2007; Kono et al., 2012). These compounds exhibit large charge carrier mobility and excellent stability. Among the donor groups, diphenylamine and its derivatives have displayed promising properties in the development of dye sensitized solar cells. Also, the carboxylic function is normally used as the electron acceptor group for the attachment of the dye on the TiO<sub>2</sub> surface (Lee, 2011; Shang, 2010). The use of  $\pi$ -conjugated systems based on thienopyrazine is selected for qualities that present the thienopyrazine ring (Campos et al., 2005; Nietfeld et al., 2011). Knowledge about the opto-electronic properties of these new materials can help with the design of new materials with optimized properties for solar energy conversion.

In what follows, theoretical study by using the DFT method on eleven conjugated compounds based on thienopyrazine, as shown in Fig. 1 is reported. Different electron side groups

**Table 1** Energy values of  $E_{LUMO}$  (eV),  $E_{HOMO}$  (eV),  $E_{gap}$  (eV) and the open circuit voltage  $V_{oc}$  (eV) of the studied molecules obtained by B3LYP/6-31G (d, p) level.

Studied compounds	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	$E_{gap}$ ( $E_{LUMO}-E_{HOMO}$ )	$V_{oc}$ (eV)/PCBM	$V_{oc}$ (eV)/TiO <sub>2</sub>
P1	-4.912	-3.085	1.827	0.912	0.706
P2	-4.943	-3.109	1.834	0.943	0.741
P3	-4.792	-2.919	1.873	0.792	0.59
P4	-4.901	-3.003	1.898	0.901	0.949
P5	-5.045	-3.099	1.946	1.045	0.803
P6	-5.038	-3.083	1.955	1.038	0.836
P7	-5.035	-3.064	1.971	1.035	0.833
P8	-5.042	-3.068	1.974	1.042	0.84
P9	-5.077	-3.075	2.002	1.077	0.875
P10	-5.095	-3.091	2.004	1.095	0.893
P11	-5.236	-3.078	2.158	1.236	1.125
PCBM*	-6.100	-3.700			
TiO <sub>2</sub> **		-3.900			

\* Wu, et al. (2010).

\*\* Tian, et al. (2010).

**Table 2** Absorption spectrum data obtained by TDDFT methods for the title compounds at B3LYP/6-31G (d, p) optimized geometries.

Compounds	Electronic transitions	$\lambda_{\text{abs}}$ (nm)	$E_{\text{ex}}$ (eV)	O.S	MO/character
P1	$S_0 \rightarrow S_1$	754.80	1.6426	0.9019	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	581.88	2.1308	0.0338	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	503.54	2.4623	0.3827	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_4$	440.39	2.8153	0.1716	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	422.54	2.9343	0.7095	HOMO $\rightarrow$ LUMO+2
	$S_0 \rightarrow S_6$	414.34	2.9923	0.1287	HOMO-1 $\rightarrow$ LUMO+1
P2	$S_0 \rightarrow S_1$	728.41	1.7021	1.0359	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	545.72	2.2719	0.0089	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	492.31	2.5184	0.3073	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_4$	455.15	2.7240	0.2893	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	438.89	2.8249	0.4223	HOMO $\rightarrow$ LUMO+2
	$S_0 \rightarrow S_6$	419.47	2.9558	0.0010	HOMO-5 $\rightarrow$ LUMO
P3	$S_0 \rightarrow S_1$	719.93	1.7222	0.7927	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	527.93	2.3485	0.0986	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_3$	486.00	2.5511	0.2519	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	435.37	2.8478	0.0838	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	411.88	3.0102	0.0201	HOMO-5 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	402.41	3.0810	0.3615	HOMO $\rightarrow$ LUMO+2
P4	$S_0 \rightarrow S_1$	699.43	1.7726	0.8707	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	576.19	2.1518	0.0685	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	489.35	2.5336	0.2596	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_4$	466.82	2.6559	0.1402	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	449.64	2.7574	0.1980	HOMO $\rightarrow$ LUMO+2
	$S_0 \rightarrow S_6$	420.31	2.9498	0.0030	HOMO-6 $\rightarrow$ LUMO
P5	$S_0 \rightarrow S_1$	698.79	1.7743	0.8569	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	514.71	2.4088	0.1080	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_3$	478.85	2.5892	0.2565	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	436.26	2.8420	0.1273	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	429.63	2.8858	0.0590	HOMO-3 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	417.56	2.9692	0.0522	HOMO-6 $\rightarrow$ LUMO
P6	$S_0 \rightarrow S_1$	685.26	1.8093	0.8200	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	558.89	2.2184	0.0366	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	480.31	2.5813	0.2711	HOMO-4 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	460.91	2.6900	0.1418	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	432.26	2.8683	0.2614	HOMO $\rightarrow$ LUMO+2
	$S_0 \rightarrow S_6$	420.23	2.9504	0.0024	HOMO-6 $\rightarrow$ LUMO
P7	$S_0 \rightarrow S_1$	686.18	1.8069	0.9294	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	519.49	2.3867	0.0008	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	509.60	2.4330	0.0925	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	475.90	2.6052	0.2388	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_5$	438.94	2.8246	0.1105	HOMO-3 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	417.93	2.9666	0.0074	HOMO-6 $\rightarrow$ LUMO
P8	$S_0 \rightarrow S_1$	684.35	1.8117	0.9391	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	508.16	2.4399	0.0920	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	475.23	2.6089	0.2363	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_4$	439.48	2.8212	0.1142	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	418.72	2.9610	0.0094	HOMO-6 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	406.08	3.0532	0.5567	HOMO $\rightarrow$ LUMO+2
P9	$S_0 \rightarrow S_1$	683.31	1.8145	0.8348	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	504.39	2.4581	0.1172	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_3$	473.88	2.6163	0.2448	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	429.70	2.8854	0.1437	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	418.33	2.9638	0.0229	HOMO-6 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	401.65	3.0869	0.3203	HOMO $\rightarrow$ LUMO+2

**Table 2** (continued)

Compounds	Electronic transitions	$\lambda_{\text{abs}}$ (nm)	$E_{\text{ex}}$ (eV)	O.S	MO/character
P10	$S_0 \rightarrow S_1$	674.20	1.8390	0.9456	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	497.58	2.4917	0.1353	HOMO-2 $\rightarrow$ LUMO
	$S_0 \rightarrow S_3$	479.33	2.5866	0.0077	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	470.74	2.6338	0.2181	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_5$	432.16	2.8690	0.1100	HOMO-3 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	419.61	2.9547	0.0147	HOMO-6 $\rightarrow$ LUMO
P11	$S_0 \rightarrow S_1$	618.44	2.0048	0.5168	HOMO $\rightarrow$ LUMO
	$S_0 \rightarrow S_2$	465.57	2.6631	0.2511	HOMO $\rightarrow$ LUMO+1
	$S_0 \rightarrow S_3$	456.02	2.7189	0.1814	HOMO-1 $\rightarrow$ LUMO
	$S_0 \rightarrow S_4$	417.87	2.9670	0.0040	HOMO-4 $\rightarrow$ LUMO
	$S_0 \rightarrow S_5$	399.43	3.1040	0.0080	HOMO-3 $\rightarrow$ LUMO
	$S_0 \rightarrow S_6$	386.59	3.2071	0.1232	HOMO-2 $\rightarrow$ LUMO

were introduced to investigate their effects on the electronic structure; The HOMO, LUMO and Gap energy of these compounds have been calculated and reported in this paper. A systematic theoretical study of such compound has not been reported as we know. Thus, our aim is first, to explore their electronic and spectroscopic properties on the basis of the DFT quantum chemical calculations. Second, we are interested to elucidate the parameters that influence the photovoltaic efficiency toward better understanding of the structure–property relationships. We think that the structural, electronic and optical properties for these compounds could help to design more efficient functional photovoltaic organic materials.

## 2. Theoretical methodology

All molecular calculations were performed in the gas phase using Density Functional Theory (DFT) using the B3LYP (Becke three-parameter Lee–Yang–Parr) exchange correlation functional (Becke, 1993; Ditchfield et al., 1971). The basis set 6-31G (d, p) was used for all atoms. All the optimizations were done without constraint on dihedral angles. The ground state energies and oscillator strengths were investigated using TD-DFT calculations on the fully DFT optimized geometries. The calculations were carried out using the Gaussian 09 program (Frisch et al., 2003). All calculations on the studied compounds of this work were done on cluster machines in the IPREM of Pau in France.

## 3. Results and discussion

### 3.1. Geometric and electronic properties

The sketch map of studied structures is depicted in Fig. 1 and the optimized geometries obtained by B3LYP/6-31G (d, p) of the studied molecules are plotted in Fig. 2. Table 1 lists the theoretical electronic property parameters ( $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and Gap). Calculated band gaps were in the range of 1.8–2.2 eV.

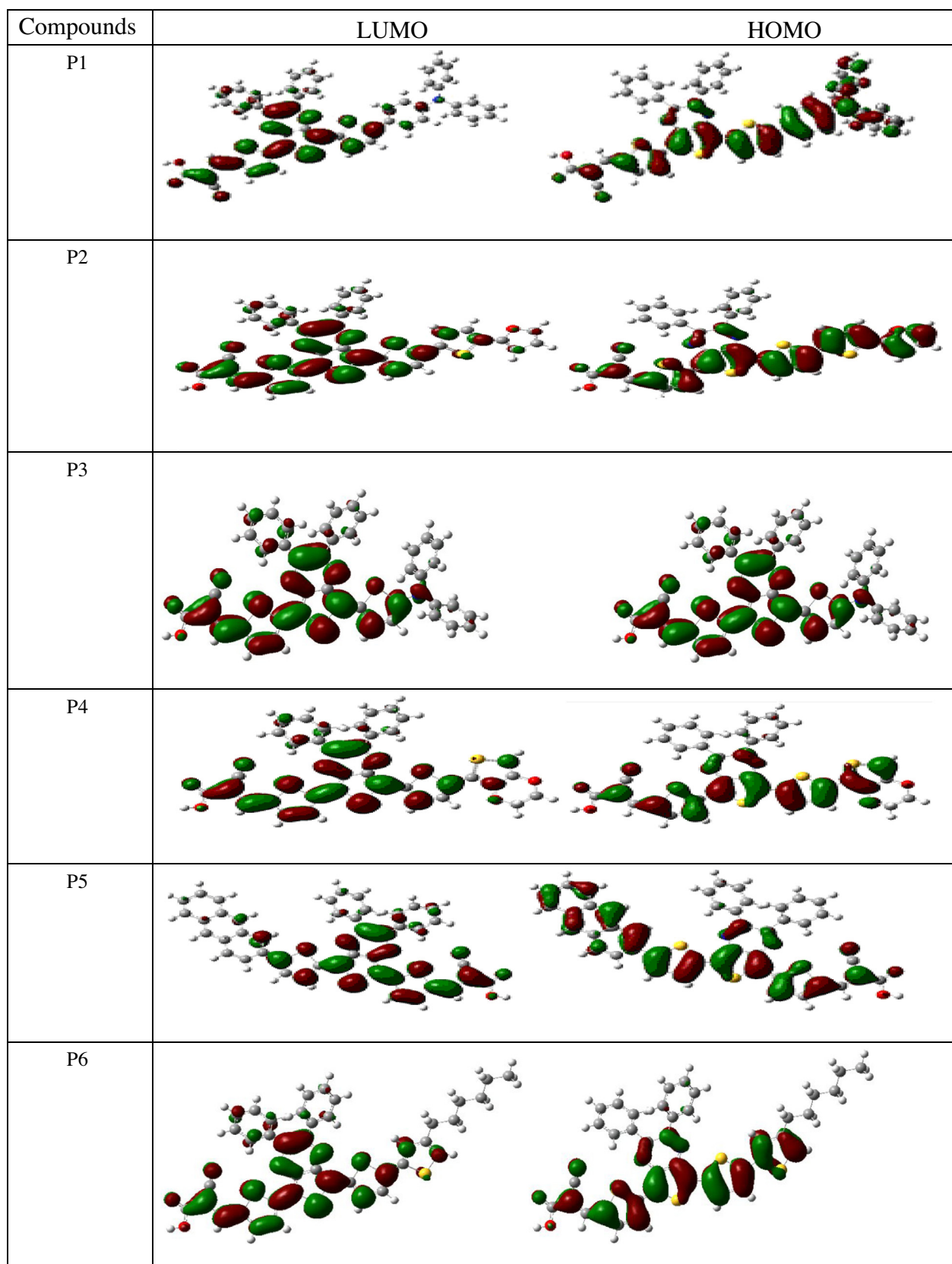
The calculated parameters (HOMO, LUMO, Gap) of, P1, P2, P3, P4, P5, P6, P7, P8, P9, P10 and P11 are (–4.912, –4.943, –4.792, –4.901, –5.045, –5.038, –5.035, –5.042, –5.077, –5.095, –5.236, –6.030 eV), (–3.085, –3.109, –2.919, –3.003, –3.099, –3.083, –3.064, –3.068, –3.075,

–3.091, –3.078 eV) and (1.827, 1.834, 1.873, 1.898, 1.946, 1.955, 1.971, 1.974, 2.002, 2.004, 2.158 eV)), respectively.

The calculated band gap  $E_{\text{gap}}$  of the studied compound increases in the following order P1 < P2 < P3 < P4 < P5 < P6 < P7 < P8 < P9 < P10 < P11. Table 1 shows detailed data of absolute energy of the frontier orbital for the studied molecules Pi and [6,6]-phenyl-C<sub>61</sub>-butyric acid methyl ester named PCBM and TiO<sub>2</sub> are included for comparison purposes. It is deduced that the modification of structure pushes up/down the HOMO/LUMO energies in agreement with their electron donor/acceptor character. To evaluate the possibilities of electron transfer from the excited studied molecules to the conductive band of the acceptor ([6,6]-phenyl-C<sub>61</sub>-butyric acid methyl ester (PCBM) or TiO<sub>2</sub>) the HOMO and LUMO levels were compared (Fig. 3). Generally, the most efficient material solar cells are based on the bulk hetero-junction structure of the blend of  $\pi$ -conjugated molecule or polymer donors and fullerene derivative acceptors (Gunes et al., 2007; Dennler et al., 2009). Here, we studied the photovoltaic properties of the compounds Pi as donor blended with [6,6]-phenyl-C<sub>61</sub>-butyric acid methyl ester (PCBM) or TiO<sub>2</sub>, which are the most broadly used as an acceptor in solar cell devices.

The HOMO and the LUMO energy levels of the donor and acceptor components are very important factors to determine whether effective charge transfer will happen between donor and acceptor. As shown in Table 1, the change of the electron-donor shows a great effect on the HOMO and LUMO levels. The experiment phenomenon was quite consistent with the previous literature (Derouiche and Djara, 2007; Zhang et al., 2008). When we compare these results with those of inorganic materials there they are very close, while in other cases the inorganic materials seem better for the manufacture of solar-paneled cells (Geng et al., 2010; Miles et al., 2007).

It is important to note that the LUMO levels of the studied compounds are higher than those of the conduction band of the acceptor PCBM or TiO<sub>2</sub> (Table 2). The difference in the LUMO energy levels of the studied compounds Pi and the acceptor is in the range of 1.710–1.266 eV (or 1.125–0.590 eV), suggesting that the photoexcited electron transfer from Pi to PCBM (or from Pi to TiO<sub>2</sub>) may be sufficiently efficient to be useful in photovoltaic devices (Xu et al., 2009). On the other hand and knowing that in organic solar cells, the open circuit voltage is found to be linearly dependent on the



**Figure 4** The contour plots of HOMO and LUMO orbitals of the studied compounds Pi.

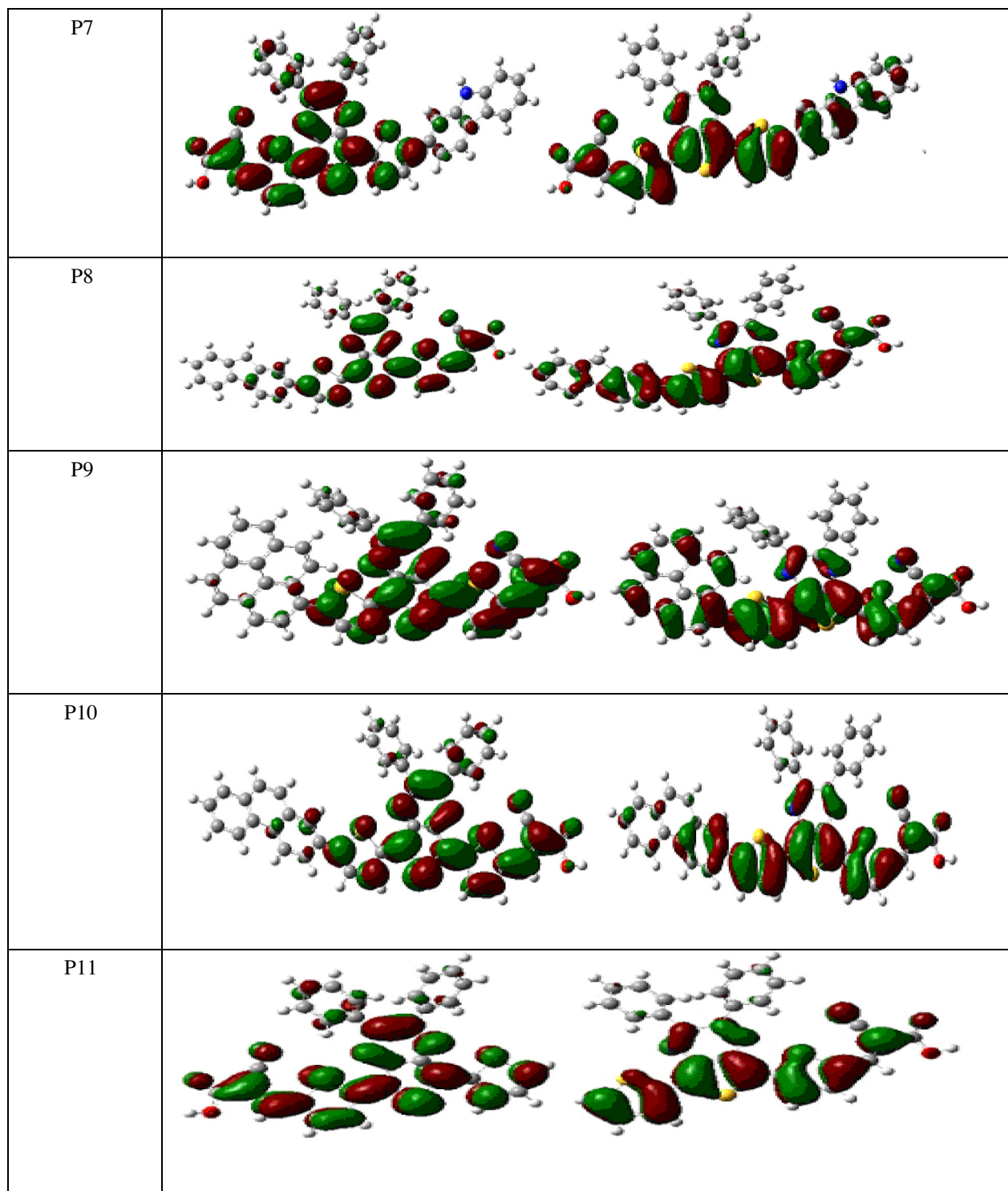


Fig. 4 (continued)

HOMO level of the donor and the LUMO level of the acceptor (Gadisa et al., 2004; Scharber et al., 2006). The power conversion efficiency ( $P_{CE}$ ) was calculated according to the following Eq. (1):

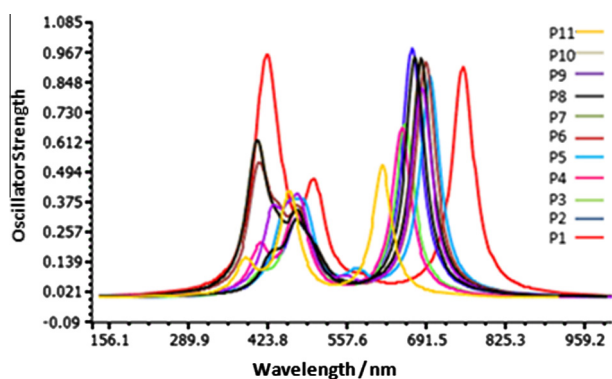
$$P_{CE} = 1/P_{in}(FF \cdot V_{oc} \cdot J_{sc}) \quad (1)$$

where  $P_{in}$  is the incident power density,  $J_{sc}$  is the short-circuit current,  $V_{oc}$  is the open-circuit voltage, and FF denotes the fill factor.

The maximum open circuit voltage ( $V_{oc}$ ) of the Bulk Hetero Junction solar cell is related to the difference between the highest occupied molecular orbital (HOMO) of the electron donor and the LUMO of the electron acceptor, taking into account the energy lost during the photo-charge generation (Wu et al., 2010). The theoretical values of open-circuit voltage  $V_{oc}$  have been calculated from the following expression (2):

$$V_{oc} = |E_{HOMO}(\text{Donnor})| - |E_{LUMO}(\text{Acceptor})| - 0.3 \quad (2)$$





**Figure 5** Simulated UV-visible optical absorption spectra of title compounds with the calculated data at the TDDFT/B3LYP/6-31G(d, p) level.

The theoretical values of the open circuit voltage  $V_{oc}$  of the studied molecules range from 1.266 eV to 1.710 eV in the case of PCBM (Table 1), these values are sufficient for a possible efficient electron injection. Therefore, all the studied molecules can be used as sensitizers because the electron injection process from the excited molecule to the conduction band of the acceptor (PCBM) and the subsequent regeneration is possible in organic sensitized solar cell.

The frontier molecular orbital (MO) contribution is very important in determining the charge-separated states of the studied molecules because the relative ordering of occupied and virtual orbital provides a reasonable qualitative indication of excitation properties and provides also the ability of electron hole transport. The iso-density plots of the model compounds are shown in Fig. 4. In general, and as plotted in this figure the HOMO possesses an anti-bonding character between the consecutive subunits. On the other hand, the LUMO of all studied compounds generally shows a bonding character between the subunits.

### 3.2. Absorption properties

How the absorption of a new material matches with the solar spectrum is an important factor for the application as a photovoltaic material, and a good photovoltaic material should have broad and strong visible absorption characteristics. From the optimized structure obtained with the method B3LYP/6-31G(d, p) of each studied compound, we have calculated the UV-Vis spectra of the studied molecules  $P_i$  using the TD/DFT method. The corresponding simulated UV-Vis absorption spectra of  $P_i$ , presented as oscillator strength against wavelength, are shown in Fig. 5. As illustrated in Table 2, we can find the values of calculated absorption  $\lambda_{max}$  (nm) and oscillator strength (O.S) along with main excitation configuration of the studied compounds  $P_i$ .

The calculated wavelength  $\lambda_{abs}$  of the studied compounds decreases in the following order  $P1 > P2 > P3 > P4 > P5 > P7 > P6 > P8 > P9 > P10 > P11$  which is the same order of the reduction of the acceptor strength. This bathochromic effect from P11 to P1 is obviously due to increased  $\pi$  delocalization. This interesting point is seen both by analyzing electronic and absorption results. Excitation to the  $S_1$  state corresponds exclusively to the promotion of an electron from

the HOMO to the LUMO. The absorption wavelengths arising from  $S_0 \rightarrow S_1$  electronic transition increase progressively with the increasing of conjugation lengths. It is reasonable, since HOMO  $\rightarrow$  LUMO transition is predominant in  $S_0 \rightarrow S_1$  electronic transition; the results are a decrease of the LUMO and an increase of the HOMO energy.

## 4. Conclusion

In this study, we have used the DFT DFT/B3LYP method to investigate theoretical analysis on the geometries and electronic properties of some thienopyrazine-derivatives in alternate donor-acceptor structure. The modification of chemical structures can greatly modulate and improve the electronic and optical properties of pristine studied materials. The electronic properties of new conjugated materials based on thienopyrazine and heterocyclic compounds and different acceptor moieties have been computed using 6-31G(d, p) basis set at density functional B3LYP level, in order to guide the synthesis of novel materials with specific electronic properties. The concluding remarks are:

- The UV-Vis absorption properties have been obtained by using TD/DFT calculations. The obtained absorption maximums are in the range of 755–618 nm.
- The HOMO level, LUMO level, and band gap of the studied compounds were well controlled by the acceptor strength. The calculated band gap  $E_{gap}$  of the studied molecules was in the range of 1.827–2.158 eV
- The calculated values of  $V_{oc}$  of the studied molecules range from 1.266 eV to 1.710 eV in the case of PCBM, these values are sufficient for a possible efficient electron injection

These obtained values are sufficient for a possible efficient electron injection. Therefore, all the studied molecules can be used as sensitizers because the electron injection process from the excited molecule to the conduction band of the acceptor (PCBM) and the subsequent regeneration is possible in organic sensitized solar cell.

The theoretical results suggest that both the acceptor strength and the stable geometry contribute significantly to the electronic properties of alternating donor-acceptor conjugated copolymers. Finally, the procedures of theoretical calculations can be employed to predict the electronic properties on the other compounds, and further to design novel materials for organic solar cells.

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