

Investigations of the Bridged Thiophene Derivative Effect on the Performance of *N,N*-diethylaniline-based Compounds for Organic Photovoltaic Cells

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Abstract:

In this work, we study eight novel organic donor- π -acceptor dyes (P_i ($i=1-8$)), used for dye sensitized solar cells (DSSCs). The designed dyes are differentiated by the nature of the π -bridge linked the electron donor group *N,N*-diethylaniline and the acceptor cyanoacrylic acid group. In this study Density Functional Theory (DFT) and its extensible Time Dependent DFT (TDDFT) approaches have been used to shed light on how the π -conjugation order influence the performance of the dyes in the DSSCs. The HOMO, LUMO and Gap energy of these compounds have been calculated and reported in this paper. Our aim is to explore their electronic and optoelectronic properties based on the DFT quantum chemical calculations. Also, we were interested to elucidate the parameters that influence the photovoltaic efficiency toward better understanding of the structure-property relationships. The study of the electronic and optical properties of these compounds could help design more efficient organic photovoltaic functional materials.

Keywords: DFT calculations; *N,N*-diethylaniline-based compounds; optoelectronic properties; organic solar cell

1. Introduction

The research of new materials based on π -conjugated molecules have become one of the most interesting topics in the chemistry, physics and material science fields. Due to their specific properties, these compounds become the most promising materials for the optoelectronic device technology [1-3], such as LEDs [4], Transistors (TFTs) [5] and solar cells [6-7].

Many researchers have been interested in synthesizing short chain compounds based on conjugated molecules because they are not amorphous and can be synthesized as well-defined structures [8-12]. On the other hand, since the discovery of the ultra-fast and ultra-efficient

photo induced electron transfer between π -conjugated systems and fullerene derivatives [13-14], a considerable interest for hetero-junction solar cells based on interpenetrating networks of conjugated systems and C60 derivatives have been generated [15]. Roquet and all reported the relationships between the natures of acceptor groups in the molecule and the photovoltaic performance [16]. 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

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increasing its efficiency [17]. The control of this parameter of these materials is a research issue of ongoing interest. Furthermore, the band gap engineering gives this material its desired electrical and optical properties. However, the most efficient strategy has been applied to design molecules that alternate donor–acceptor repeating units that are expected to have small gaps [18].

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. There by contributing to the rationalization of the properties of known materials and the prediction of those yet unknown [19-23].

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 highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels of the components is basic in studying organic solar cells. So, we can save time and money by predicting theoretical the adequate organic materials for photovoltaic devices. 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 of HOMO and LUMO levels will prove responsible for the improvement of all photovoltaic properties of the organic solar cells.

Recently, the compounds with donor- π -conjugated-acceptor (D- π -A) structure is described and studied by different authors who have shown the importance of these materials in use as a solar cell [24-28]. These compounds exhibit large charge carrier mobility and excellent stability. Among the donor groups, the *N,N*-diethylaniline and its derivatives take our interest, which was less explored in the development of dye sensitized solar cells. However, the carboxylic function is normally used as the electron acceptor group for the attachment of the conjugate molecules on the acceptors [29]. The use of π -conjugated systems, linked the donors and acceptors parts, based on thiophene derivatives

are selected for qualities that present the thiophene derivatives ring [30-33]. 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 eight conjugated compounds incorporate thiophene derivatives as π -conjugate linked the electron donor group *N,N*-diethylaniline and the acceptor cyanoacrylic acid group, as shown in Figure 1. The different thiophene derivatives (π -conjugated systems) were introduced to investigate their effects on the performance of their resulted organic photovoltaic cells. The HOMO, LUMO and Gap energy of the resulted 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 spectral properties using DFT quantum chemical calculations. Second, we are interested to elucidate the parameters that influence the photovoltaic efficiency toward better understanding of the structure–properties relationship. We think that the electronic and optical properties of these compounds could help to design more efficient functional photovoltaic organic materials.

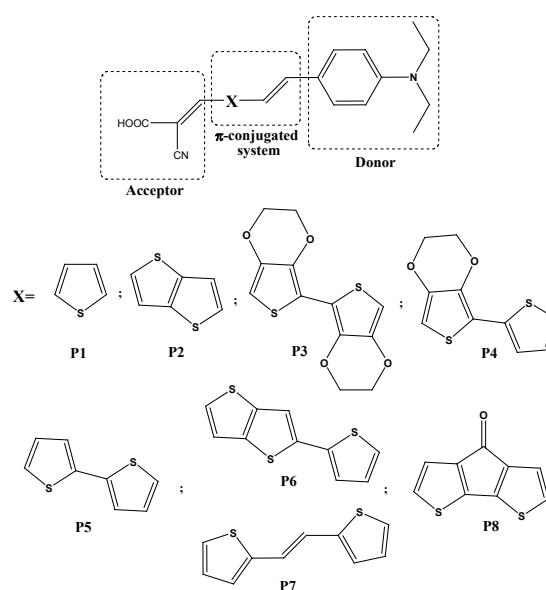


Figure 1. Chemical structure of study compounds P_i ($i = 1-8$).

2. Results and Discussion

2.1. Geometries and electronic properties

The sketch map of designing molecular

structures (Figure 1) was optimized at their ground state geometries by B3LYP/6-31G(d,p) level and presented in Figure 2.

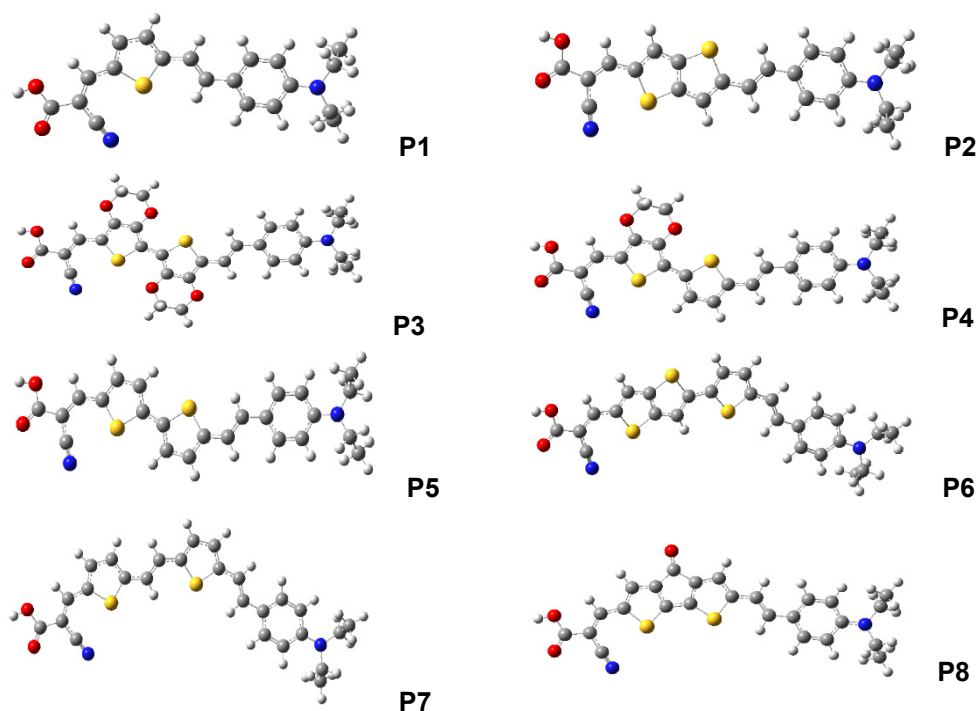


Figure 2. Optimized geometries obtained by B3LYP/6-31G(d,p) of the studied compounds.

The electron/hole transfer and electron injection performance depends essentially on the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), Gap energy (E_{gap}), Ionization Potentials (IP) and Electron Affinities (EA) parameter values. For a better understanding of the electronic properties of the studied dyes, we illustrate the band structure diagram of the HOMOs and LUMOs energies in Figure 3. The calculated values of the HOMOs, LUMOs, IP, and EA were presented in Table 1, with the open-circuit voltage (V_{oc}) value (which is the maximum possible voltage across a photovoltaic cell in sunlight when no current from flowing) for the conjugated compounds (as donors) blended with PCBM (as acceptor).

As shown in Table 1 the neutral state the band gaps were calculated in the range of 1.922–2.515 eV. However, the calculated parameters (HOMO, LUMO, Gap) of P1, P2, P3, P4, P5, P6, P7 and P8 are (-5.028, -4.783, -5.018, -4.842, -4.853, -

4.728, -4.562, -4.991 eV), (-2.513, -2.666, -2.605, -2.689, -2.638, -2.479, -2.307, -3.079 eV) and (2.515, 2.117, 2.413, 2.153, 2.215, 2.248, 2.255, 1.922 eV)), respectively.

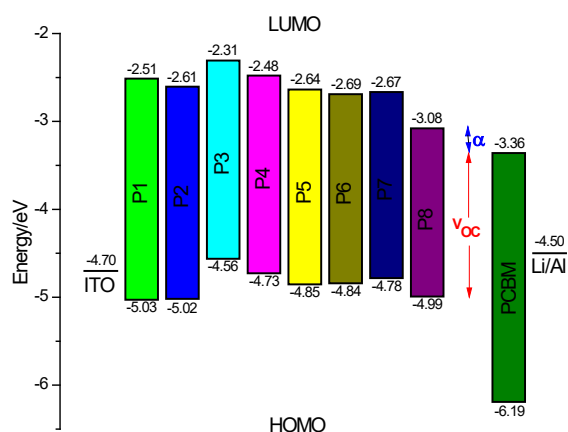


Figure 3. Band structure diagram illustrating the HOMO and LUMO energies of P_i with $i = 1-8$ relative to the band structure of PCBM.

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

Compounds	E_{HOMO}	E_{LUMO}	E_{gap}	PI	AE	V_{oc} /PCBM	α^*
P1	-5.028	-2.513	2.515	6.159	1.351	1.368	0.847
P2	-5.018	-2.605	2.413	6.067	1.519	1.358	0.755
P3	-4.562	-2.307	2.255	5.489	1.329	0.902	1.053
P4	-4.728	-2.479	2.248	5.699	1.459	1.068	0.881
P5	-4.853	-2.638	2.215	5.879	1.570	1.193	0.722
P6	-4.842	-2.689	2.153	5.811	1.677	1.182	0.671
P7	-4.783	-2.666	2.117	5.741	1.672	1.123	0.694
P8	-4.991	-3.079	1.922	5.987	2.036	1.331	0.281
PCBM [34]	-6.190	-3.360					

* $\alpha_i = E_{LUMO}(P_i) - E_{LUMO}(PCBM)$; $i=1$ to 8.

The calculated band gap E_{gap} of the studied compound decreases in the following order $P1 > P2 > P3 > P4 > P5 > P6 > P7 > P8$, suggest a red shift of the absorption spectra of these compounds in the same order.

The adequate and balanced transport of both injected electrons and holes is important in optimizing the performance of electronic devices. The ionization potential (IP) and electron affinity (EA) is well-defined properties that can be calculated by the DFT to estimate the energy barrier for the injection of both holes and electrons. The IP and EA have been calculated as follows:

$$IP = E^+(M^+) - E(M)$$

$$EA = E(M) - E^-(M^-)$$

here, $E(M)$ and $E^+(M^+)$ represent the energies of the neutral and cation species in their lowest energy geometries, respectively, while $E^-(M^-)$ represent the energies of the anionic specie in their lowest energy geometry. It is advantageous for the generation of free electrons based on the lower IP, and the generation of free hole based on the higher EA, as the augmentation of p-type materials in organic solar cell devices [35]. As shown in Table 1, the calculated IP decreases in the following order: $P1 > P2 > P8 > P5 > P6 > P7 > P4 > P3$ indicate that P3 dye is suitable to generate free electrons compared to the other investigated dyes. While the calculated EA increase as follows: $P1 < P3 < P4 < P2 < P5 < P7 < P6 < P8$, suggests that P8

dye is suitable to generate free holes than the other studied compounds.

Generally, efficient materials for solar cells are based on the bulk hetero-junction structure of the blend of π -conjugated molecule or polymer donors and fullerene derivative acceptors [36, 37]. Here, we studied the photovoltaic properties of the compounds P_i as donor blended with PCBM, which are the most broadly used as an acceptor in solar cell devices.

It is important to note that the LUMO levels of the studied compounds are higher than the conduction band of the acceptor TiO_2 (Table 1). The difference in the LUMO energy levels of the studied compounds P_i and the acceptor (α) is in the range of 0.281–1.053 eV suggesting that the photoexcited electron transfer from P_i to PCBM may be sufficiently efficient to be useful in photovoltaic devices [38]. On the other hand and knowing that in organic solar cells, the open circuit voltage is found to be linearly dependent on the HOMO level of the donor and the LUMO level of the acceptor [39]. 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 [40]. The theoretical values of open-circuit voltage V_{oc} have been calculated from the following expression:

$$V_{OC} = \left| E_{HOMO}^{(Donor)} \right| - \left| E_{LUMO}^{(Acceptor)} \right| - 0.3$$

The calculated values of the V_{oc} parameter shown in Table 1 for our investigated compounds blended with the acceptors PCBM range from (0.902 to 1.368 eV). These calculated values are sufficient for a possible efficient electron injection into LUMO of the acceptor.

2.2. Frontier molecular orbitals

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 the ability of electron hole transport. The iso-density plots of the model compounds are shown in

Figure 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. Also, in the HOMOs state the electron density of our molecules is mostly localized around the electron-donating *N,N*-diethylaniline and thiophenes bridge groups. However, in the LUMO state the electrons are localized near the electron acceptor group (cyanoacrylic acid). This indicates that the electron should move from donor to acceptor after the light absorption through excitation, and the advantageous asymmetric D-A structure favors the direct intramolecular electron transfer from donor to acceptor.

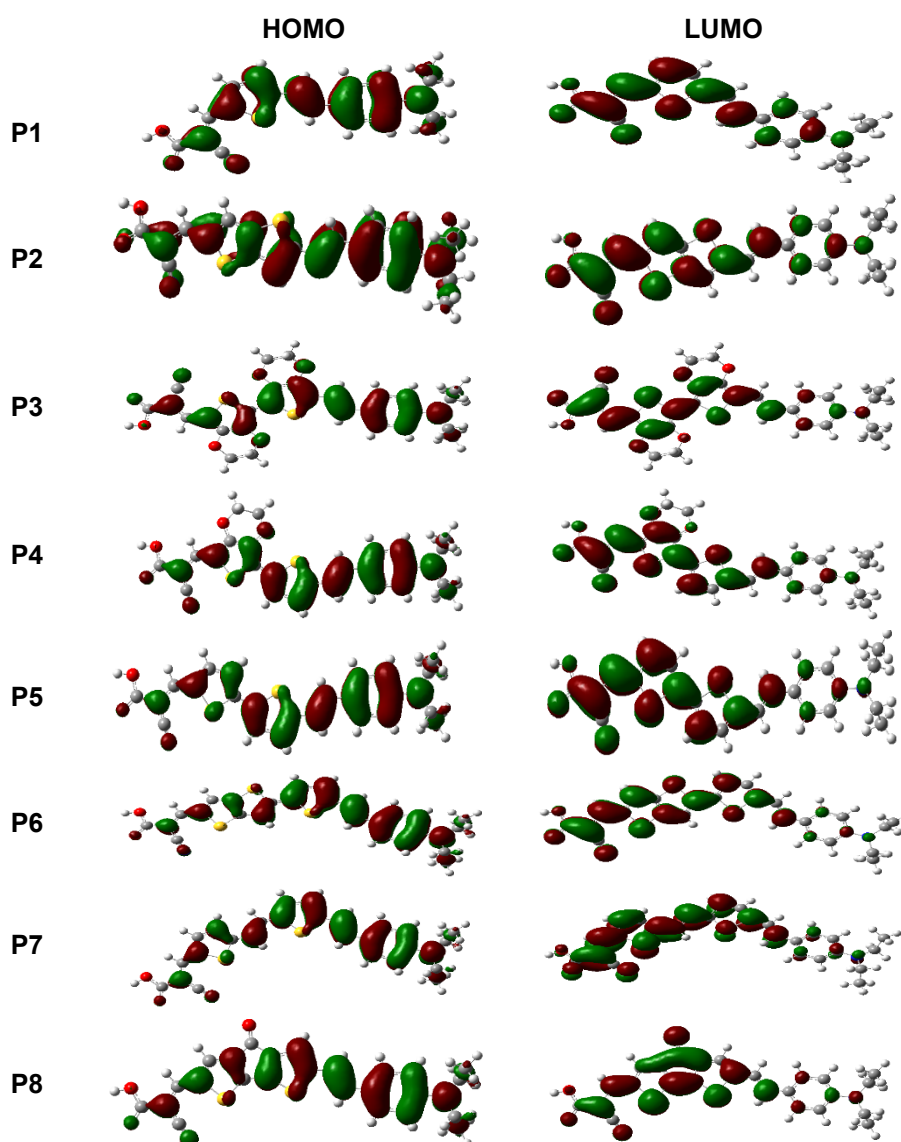


Figure 4. Isodensity plots of the frontier orbitals of the studied compounds obtained by B3LYP/6-31G(d,p).

2.3. Absorptions 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 Pi in a vacuum using the TD/DFT method. The corresponding simulated UV–Vis

absorption spectra of Pi are presented in Figure 5.

As shown in Figure 5, the absorption spectra of the studied compounds have widely and intense visible absorption, suggest that we designed compounds must absorb and convert the sunlight to electricity. As illustrated in Table 2, we can find the values of calculated absorption λ_{abs} (nm) and oscillator strength (O.S) along with the main excitation configuration of the studied compounds Pi.

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

Compounds	Electronic transitions	λ_{abs} (nm)	E_{ex} (eV)	O. S	MO/character*
P1	$S_0 \rightarrow S_1$	511.3	2.42	1.0973	H→L(0.62)
	$S_0 \rightarrow S_2$	365.2	3.39	0.3122	H-1→L+1 (0.50)
	$S_0 \rightarrow S_3$	315.0	3.93	0.1060	H→L+1 (0.50)
P2	$S_0 \rightarrow S_1$	533.29	2.32	1.3975	H→L (0.62)
	$S_0 \rightarrow S_2$	387.16	3.20	0.6448	H-1→L (0.56)
	$S_0 \rightarrow S_3$	360.80	3.43	0.0259	H-2→L (0.66)
P3	$S_0 \rightarrow S_1$	576.22	2.15	1.4057	H→L (0.70)
	$S_0 \rightarrow S_2$	432.41	2.86	0.3840	H-1→L (0.61)
	$S_0 \rightarrow S_3$	378.63	3.27	0.1599	H→L+1(0.50)
P4	$S_0 \rightarrow S_1$	585.01	2.11	1.2448	H→L (0.70)
	$S_0 \rightarrow S_2$	427.12	2.90	0.5769	H-1→L (0.62)
	$S_0 \rightarrow S_3$	374.45	3.31	0.1147	H→L+1 (0.49)
P5	$S_0 \rightarrow S_1$	591.92	2.09	1.1780	H→L (0.63)
	$S_0 \rightarrow S_2$	425.10	2.91	0.7269	H-1→L (0.56)
	$S_0 \rightarrow S_3$	375.84	3.29	0.0818	H→L+1 (0.51)
P6	$S_0 \rightarrow S_1$	615.96	2.01	1.1705	H→L (0.70)
	$S_0 \rightarrow S_2$	446.19	2.77	0.9260	H-1→L (0.56)
	$S_0 \rightarrow S_3$	398.04	3.11	0.1601	H→L+1 (0.54)
P7	$S_0 \rightarrow S_1$	619.68	2.00	1.2306	H→L (0.63)
	$S_0 \rightarrow S_2$	455.72	2.72	0.7421	H-1→L (0.54)
	$S_0 \rightarrow S_3$	403.38	3.07	0.2554	H→L+1 (0.49)
P8	$S_0 \rightarrow S_1$	747.83	1.65	0.5748	H→L (0.68)
	$S_0 \rightarrow S_2$	518.69	2.39	0.1575	H-1→L (0.53)
	$S_0 \rightarrow S_3$	465.57	2.66	0.5325	H→L+1 (0.55)

* :H=HOMO and L=LUMO

The calculated wavelength λ_{abs} (nm) arising from $S_0 \rightarrow S_1$ electronic transition increases in the following order P1 (511.34) < P2 (533.29) < P3 (576.22) < P4 (585.01) < P5 (591.92) < P6 (615.96) < P7 (619.68) < P8 (747.83(nm)) of the

studied compounds, which is the same order of the increasing band gap energy of the donor– π –acceptor molecules. This bathochromic effect from P1 to P8 is obviously due to increased π -delocalization through π -bridge block. By

analyzing the electronic transitions for all studied molecules, the first excited transition state ($S_0 \rightarrow S_1$) is mainly attributed in major contribution to an intramolecular charge-transfer transition from the donor *N,N*-diethylaniline to the acceptor cyanoacrylic acid (HOMO \rightarrow LUMO transition, see

a density plot in Figure 4. This first transition has been occurring with high oscillator strength; resulted in maximization of the photocurrent response in the studied compounds in the following order: $P8 < P1 < P6 < P5 < P7 < P4 < P2 < P3$.

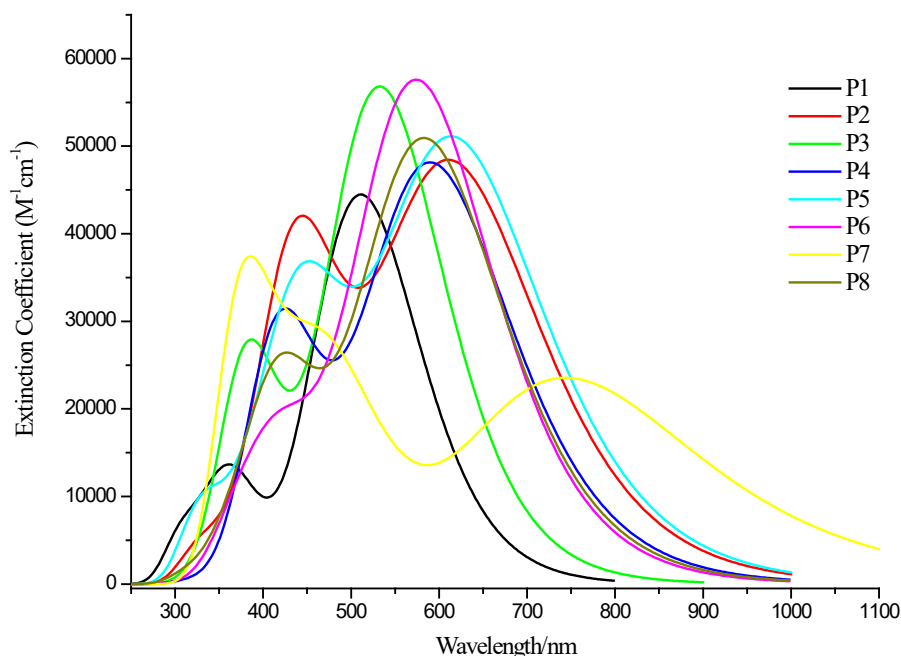


Figure 5. Simulated UV-visible optical absorption spectra of study compounds at the TD-B3LYP/6-31G(d,p) level.

3. Material and Methods

3.1 Computational methods

Full geometry optimizations at the ground and doped states were performed under no constraints in the framework of the density functional theory (DFT) by means of the B3LYP functional implemented in the Gaussian 09 program [41]. The 6-31G(d,p) basis set was chosen as a compromise between the quality of the theoretical approach and the high computational cost associated with the high number of dimensions to the problem for all atoms [42, 43]. The electronic properties such as; the HOMO and LUMO energy levels, and their gap's energies were deduced, also the Ionization Potential (IP) and Electron Affinity (EA) of the investigated molecules were calculated. In this paper, to modulate the absorption spectra, the vertical transition energies from the ground-state were calculated using TD-DFT [44, 45]

calculations in vacuum with the same functional and basis set.

4. Conclusions

In the present work, our computational results predicted the electronic and optical properties of a series of newly designed *N,N*-diethylaniline-based donor compounds linked with the acceptor cyanoacrylic acid by π -conjugated thiophene derivatives (Pi ($i=1-8$)). They were studied by means of quantum chemical method based on the DFT and TDDFT methods, using B3LYP functional and 6-31G(d,p) basis set, in order to display the effect of π -conjugated thiophene derivatives on the electronic and spectral properties of these compounds.

The concluding remarks are:

- The maximums UV-Vis absorption spectra, obtained by TDDFT calculations, are in the range

of 748–511 nm, suggest that our designed compounds must absorb and convert the sunlight to electricity.

- The HOMO, LUMO levels, and band gap energy of these compounds have raised during this study. The calculated band gap E_{gap} of the studied molecules was in the range of 1.922–2.515 eV, and resulted in decreasing order as follows: P1>P2>P3>P4>P5>P6>P7>P8, suggest a red shift of the absorption spectra of these compounds in the same order.

- The calculated IP, decrease in the following order: P1>P2>P8>P5>P6>P7>P4>P3 indicate that P3 dye is suitable to generate free electrons compared to the other investigated dyes. While the calculated EA increase as follows: P1<P3<P4<P2<P5<P7<P6<P8, suggests that P8 dye is suitable to generate free holes than the other studied compounds.

- The calculated values of V_{oc} of the studied molecules range from 0.262 to 0.728 eV in the case of, these values are sufficient for a possible efficient electron injection into the conduction band of the acceptor PCBM.

Finally, the theoretical results suggest that engineering the π -conjugated systems linked the donor and acceptor groups were contributed significantly to enhance the optoelectronic properties of the conjugated compounds. This procedure can be used to predict the optoelectronic properties of the other compounds, and further to design new active materials for organic solar cells

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