Full Paper

DFT Study of Electronic and Optical Properties of Small Oligothiophenes Based on Terthiophene End-capped by Several Donor Groups

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Abstract: Eight small molecules based on terthiophene end-capped by several donor groups have been carried out using density functional theory (DFT) and time-dependent (TDDFT) methods in neutral and doped states. The theoretical ground-state geometry, electronic structure and optical properties of the studied molecules were obtained by the DFT and TD-DFT methods at the B3LYP level with 6-31G(d) basis set. Theoretical knowledge of the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) energy levels the gap energy (Eg) and the open-circuit voltage (Voc) of the studied compounds are calculated and discussed. The effects of the donor group substituents on the geometries and optoelectronic properties of these materials are discussed to investigate the relationship between molecular structure and optoelectronic properties. The results of this work suggest some of these materials as a good candidate for organic solar cells.

Keywords: π-conjugated molecules; oligothiophenes; optoelectronic properties; DFT; TDDFT; organic solar cell

1. INTRODUCTION

Among electrically conducting polymers, π-conjugated linear polymers, such as polyacetylene, poly(p-phenylene), poly(p-phenylene vinylene), poly(phenylene sulfide), polypyrrole, , polyaniline and polythiophene, have attracted a great deal of attention because of their ability to achieve high electrical conductivity by doping[1-5]. The conjugated materials based on thiophene are very important and prospect class of organic materials for their use in organic light emitting diodes (OLEDs) [6, 7], field effect transistors (OTFTs) [9-10], lasers [11], sensors [12] and organic solar cells [13-23].

Oligothiophene have been explored as active materials for organic semiconductors due to facile chemical modification of their structures which allow fine-tuning of their optical and electrical properties. Moreover, these materials are attractive due to their low density, flexibility, environmental friendliness and processibility over large coverage areas.

To make the π-conjugated material as oligothiophene absorb more photons, it is necessary to minimize the band gap of this material to increase the photon absorption. Moreover, several other factors of these compounds including HOMO, LUMO levels, charge carrier mobility and the open-circuit voltage (Voc) which is the difference between the HOMO level of the electron-donating molecule and the LUMO level of the PCBM and its derivatives (acceptor most used in organic solar cells) should be maximized, need to be optimized simultaneously in order to achieve the desired photovoltaic performances. In addition, the LUMO level of the conjugated molecule (donor) should be positioned above the LUMO of the PCBM (acceptor) to an amount estimated to around 0.3 eV to ensure efficient electron transfer. Among the factors for enhance these properties, several substituent donor groups were attached to oligothiophene compounds for this goal.

In this work, theoretical study by using density functional theory (DFT) and time-dependent (TDDFT) methods on eight small conjugated compounds based on terthiophene end-capped by

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several electron donor groups (-H, -CH3, -O-CH3, phenyl, fluorinyl, furanyl, thiophenyl and thienylenevinylenyl). The geometry structures, electronic properties of neutral and polaronic forms and spectroscopic characteristics of these compounds have been predicted using DFT method with B3LYP/6-31G(d) calculation. The HOMO and LUMO level energies were exanimated and the gap energy is evaluated as the difference between the HOMO and LUMO energies (Egap = |E_{HOMO} − E_{LUMO}|). The open circuit voltage (Voc) is related to the difference between the HOMO of the electron donor (studied compounds) and the LUMO of the electron acceptor PCBM (([6,6]-phenyl-C61butyric

acid methyl ester). PCBM is the most broadly used as an acceptor in solar cell devices, this acceptor has the role of accepting the electrons from the donor and thus ensures charge separation, and due to its solubility in most organic solvents. Thus, and based on the optimized geometries; the ground state energies, wavelength absorption values, oscillator strengths were investigated using the TD-DFT/ B3LYP/6-31G(d) calculations. All calculations were carried out using the Gaussian 09 program. The effects of the electron donor substituents on the geometries and electronic properties of these materials were investigated and discussed.
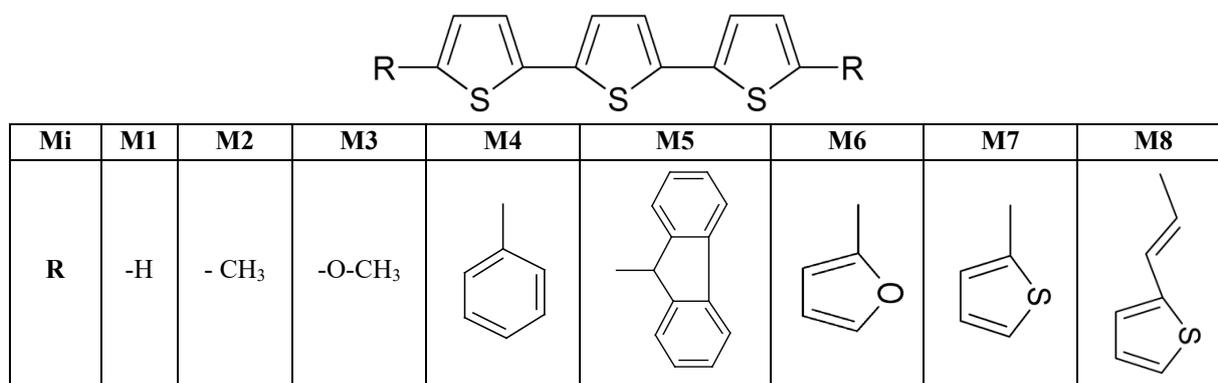

Mi	M1	M2	M3	M4	M5	M6	M7	M8
R	-H	- CH₃	-O-CH₃					

Figure 1. Chemical structures of the studied compounds M1-M8.

2. COMPUTATIONAL METHODOLOGY

The geometries and the optoelectronic properties of all molecules were calculated by Gaussian09 program supported by Gauss View 5.0 [24] using a hybrid density functional [25] and Becke's three parameter exchange functional combined with the LYP correlation functional (B3LYP) and with the 6-31G(d) basis set (B3LYP/6-31G(d)) in the gas phase. The geometry structures of neutral and doped molecules were optimized under no constraint. The HOMO, LUMO, and gap energy (which evaluated as the difference between the HOMO and LUMO energies) energies were also deduced from the optimized structures.

The vertical electronic excitation spectra, including wavelengths, oscillators strengths, and main configuration assignment, were systematically investigated using TDDFT calculations with the 6-31G (d) basis set on the fully DFT-optimized structure of the ground state [26-28]. In fact, these calculation methods have been successfully applied to other conjugated organic molecules and polymers [29].

3. RESULTS AND DISCUSSION

3.1. Structure and geometric properties

The optimized structures of the studied molecules obtained by DFT/B3LYP/ 6-31G(d) method in the ground (S0) and excited (S1) states are depicted in Fig. 3. The inter-ring bond lengths (d1 and d2) and dihedral angles (θ_1 and θ_2) of these molecules are listed in Table 1. Comparing with M1(unsubstituted molecule), in the ground states (neutral structures) it is observed that the inter-ring bond lengths d1 and d2 have a slight decrease with the end-substitution molecules by several donor groups in the order M8 < M7 < M6 < M5 < M4 < M3 < M2 < M1. Moreover, we found that the consecutive units have similar dihedral angles (the inter-ring torsions between subunits (θ_1 and θ_2)) ~180° except those of the molecules M4 and M5 have a slight torsion. This can due to the introduction of fluorine and phenyl rings for M4 and M5 respectively. In the excited states (S1) and as show in table 1, we found that the inter-ring distances d1 and d2 decrease going from the neutral structures to the excited ones and going from M1 to M8.

These results show that all studied compounds

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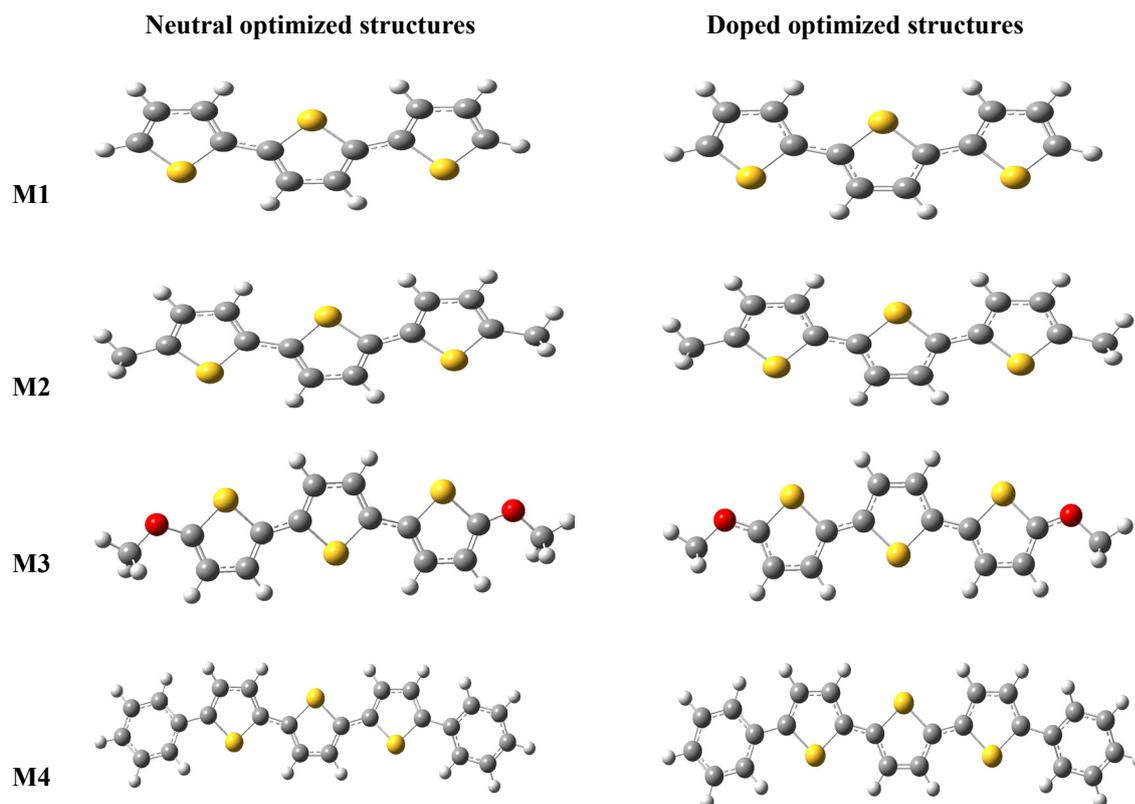*Orbital: Electron. J. Chem. 9 (3): 188-196, 2017*

have similar conformations (quasi planar conformation). We found that the adding of the substituent donor groups attached to the end terthiophene induce a slight change on the geometric parameters and favors the intramolecular charge transfer (ICT) within the molecules.
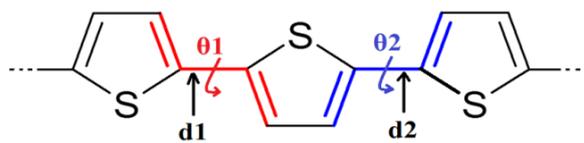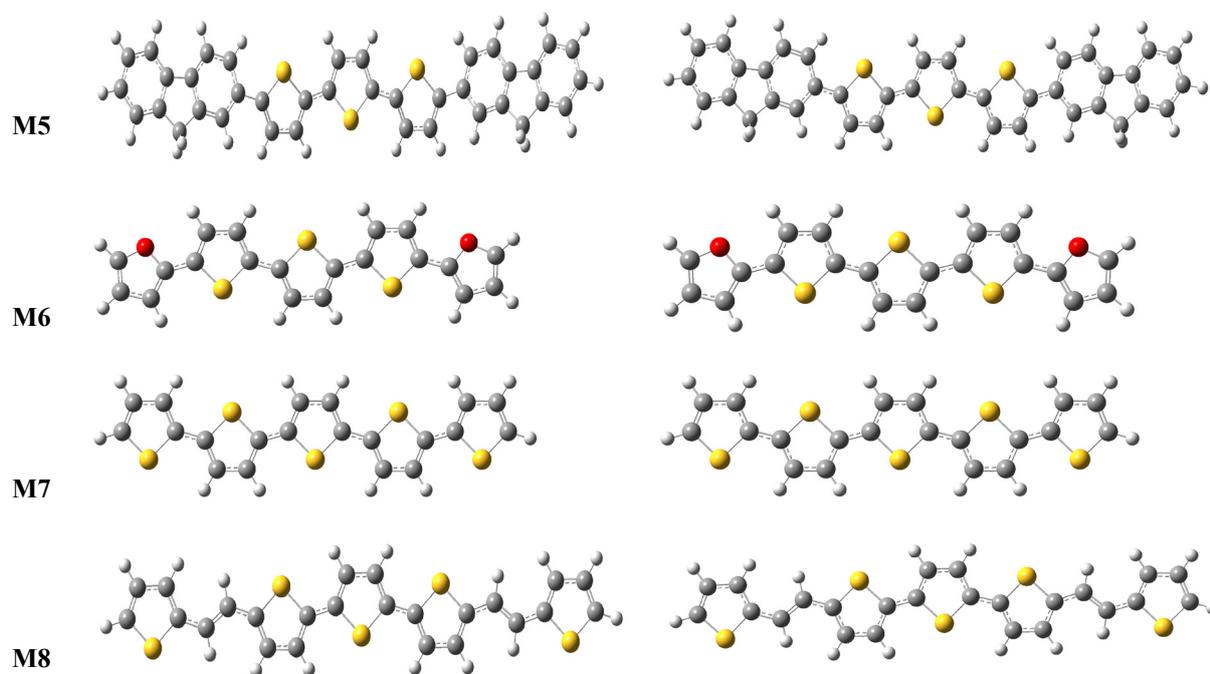

Figure 2: Geometric parameters (d1, d2, θ_1 and θ_2) in the molecules Mi (i=1...8).

Table 1: Geometric parameters of the studied compounds in the ground (neutral) and excited (polaron) states obtained by B3LYP/6-31G(d), bond lengths (Å) and dihedral angles (°).

Molecule	d_i (Å)				θ_i (°)			
	Neutral		Polaron		Neutral		Polaron	
	d_1	d_2	d_1	d_2	θ_1	θ_2	θ_1	θ_2
M1	1.4467	1.4467	1.4138	1.4138	179.97	179.99	179.99	179.99
M2	1.4454	1.4454	1.4124	1.4124	179.99	179.97	180.00	179.99
M3	1.4439	1.4439	1.4118	1.4118	179.99	179.99	179.99	179.99
M4	1.4430	1.4430	1.4112	1.4112	168.48	168.46	179.18	179.18
M5	1.4430	1.4430	1.4112	1.4112	-165.55	165.55	178.63	-178.63
M6	1.4416	1.4416	1.4112	1.4101	179.98	179.99	179.99	179.99
M7	1.4416	1.4416	1.4111	1.4111	-179.99	-179.99	-179.99	-179.99
M8	1.4404	1.4404	1.4109	1.4109	-179.94	-179.94	-179.98	-179.99

Neutral optimized structures	Doped optimized structures

M1

M2

M3

M4

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Figure 3. Optimized structures of neutral and polaronic studied molecules obtained by B3LYP/6-31G (d) level.

3.2. Optoelectronic properties

3.2.1. Frontier molecular orbitals

It's very important to examine the frontier molecular orbital (FMO) density, because this can give us information about excitation properties by indicating how the charge transfer occurred along the molecule chain. The iso-density plots of the HOMO an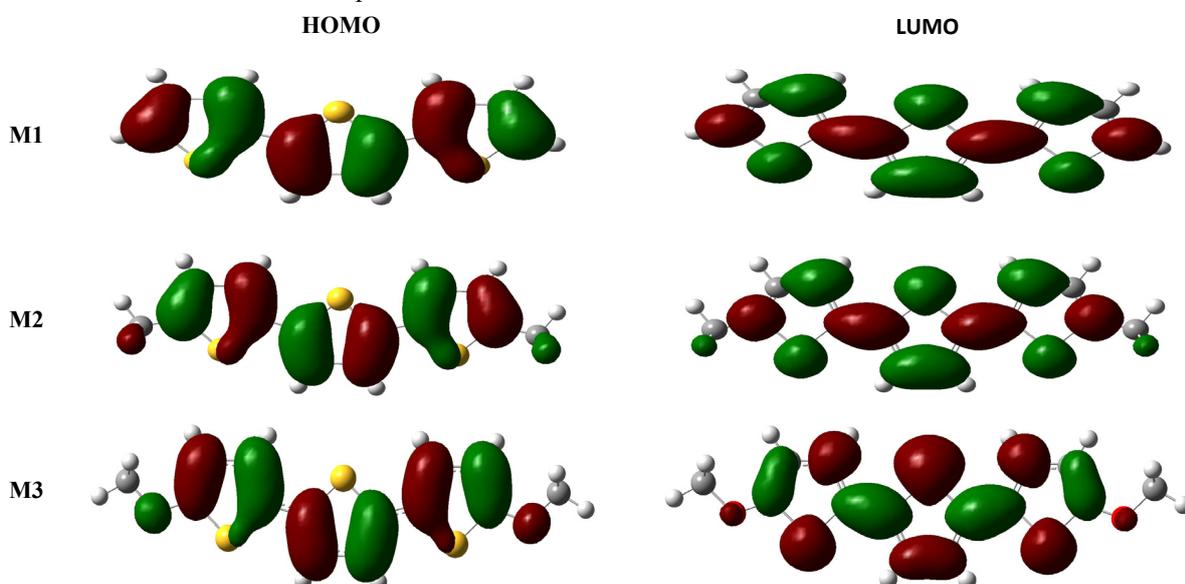d LUMO of the studied compounds are shown in Fig. 4. We note that The FMO of all compounds have analogous distribution characteristics, such as the HOMOs possess a π-bonding character within subunit and a π-antibonding character between the consecutive subunits. Whereas, the LUMO generally possess a π-antibonding character within subunit and a π-bonding character between the subunits. The HOMO and LUMO density are distributed entirely over the conjugated molecules.

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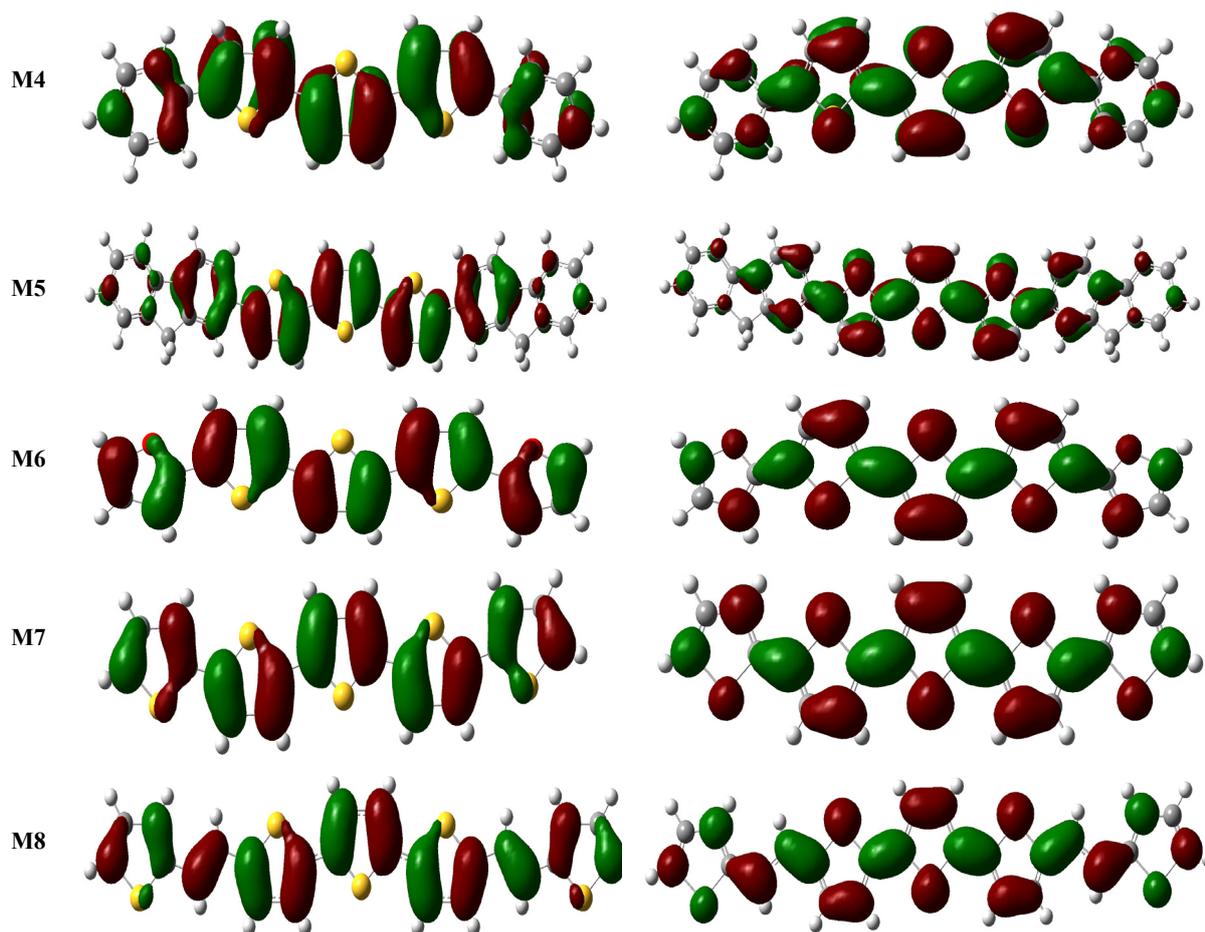
Figure 4. The contour plots of HOMO and LUMO orbital's of the neutral studied compounds.

3.2. Electronic properties

To study the electronic properties of the organic compounds used in photovoltaic cells as organic solar cells, the HOMO, LUMO band gap energies are useful parameters for this study. The HOMO and LUMO energies were obtained by DFT/B3LYP/6-31G(d) calculations, and their Data are summarized with the band gap energies of all compounds in their neutral and first excited states in Table 2. We note that the HOMO and LUMO values ranging from -4.64 to -5.14 eV and from -1.34 to -2.21 eV respectively. The LUMO values were significantly higher than that of the acceptor PCBM. Figure 5 shows the energy frontier orbitals HOMO and LUMO for the studied molecules and the conducting band levels (LUMO) of PCBM, ITO (indium tin oxide: transparent conductive oxide used as cathode) and Al (low work function metal used as anode).

The calculated Eg of the studied compounds ranges from 2.51 to 3.44 eV and decreases in the following order M1 > M2 > M3 > M4 > M5 > M6 > M7 > M8 which is the same order of increasing of the donor strength of the substituent units. Besides the donor strength, this can due to the aromaticity and the conjugated length of these units. Moreover, the smallest band gap energy has been observed for M8 (2.51 eV) with thienylenevinylene substituted groups. This can be explained by the conjugated length backbone and strong electron donor character of the thienylenevinylene.

In addition, knowing that since the p-doped, π-conjugated molecule has becomes the ultimate responsible of charged transport. The values of the energy of the HOMO, LUMO, Egap (= E_{HOMO} - E_{LUMO}) of all compounds in their neutral and polaronic forms were shown in Table 5. Comparing with the neutral and polaronic forms, we can noted clearly that the band gap energies decrease passing from the neutral to the excited forms of all studied compounds. Finally, these results clearly show the effect of the different donor substituent groups attached to the end terthiophene on the HOMO and LUMO energies on the electronic properties of these compounds.

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Table 2: Theoretical electronic properties parameters (HOMO, LUMO, Gap) obtained by B3LYP/6-31G(d) of the studied molecules.

Compounds	Ground state			Doped state		
	E_{HOMO}	E_{LUMO}	Eg	E_{HOMO}	E_{LUMO}	Eg
M1	-5.14	-1.69	3.44	-9.25	-6.12	3.12
M2	-4.93	-1.57	3.37	-8.85	-5.82	3.02
M3	-4.64	-1.34	3.29	-8.31	-5.25	2.92
M4	-4.96	-1.89	3.06	-8.15	-5.50	2.64
M5	-4.85	-1.91	2.93	-7.46	-5.05	2.41
M6	-4.78	-1.96	2.82	-7.96	-5.47	2.49
M7	-4.86	-2.08	2.78	-7.98	-5.51	2.46
M8	-4.72	-2.21	2.51	-7.48	-5.27	2.21
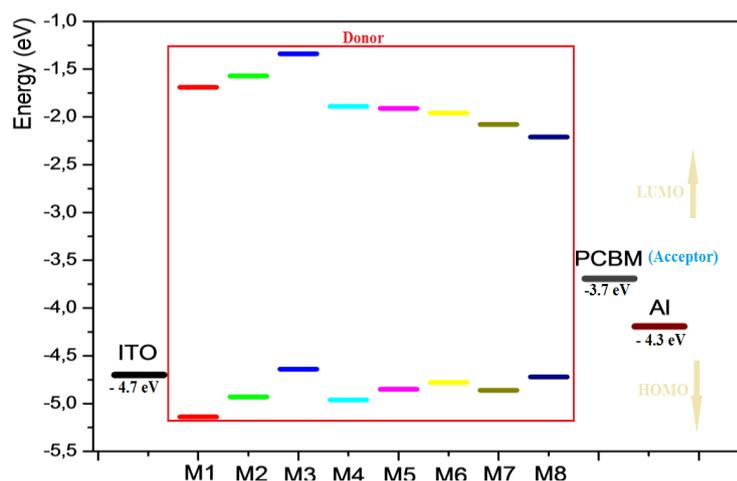
Figure 5. Data of the absolute energy of the frontier orbitals HOMO and LUMO for the studied molecules and the conducting band levels of PCBM, ITO and Al.

3.3. Photovoltaic performances

In the bulk heterojunction (BHJ) active layer , the adequate energy levels and the proper locations of HOMO and LUMO orbitales of the studied molecules are required and compared with the LUMO energy level of the electron acceptor PBCM which is most used in organic photovoltaic and solar cell devices. The highest few occupied (HOMO) and lowest few unoccupied (LUMO) orbitales are particularly interesting, since they are involved in the electron transitions, in which the photoinduced electron transfers from the excited state molecule to the electron acceptor (PBCM).

As shown in Fig.5, we noted that the LUMO levels of all studied compounds are higher than that of PCBM. So, the electron transfers from the studied molecules to the conductive band of PCBM are possible. Moreover, we note that the LUMO energy levels of the studied compounds are much higher than that of the ITO conduction band edge. Thus, all studied molecules have an ability to inject electrons

into ITO electrode.

In organic solar cells, the open circuit voltage (noted Voc which is the maximum possible voltage across a photovoltaic cell in sunlight when no current in flowing) is an important parameter to study the photovoltaic properties of these molecules (as donors) blended with PCBM (as acceptor). Voc is linearly dependent on the HOMO level of the donor and the LUMO level of the acceptor and is related to the difference between the HOMO of the electron donor (studied compounds) and the LUMO of the electron acceptor (PCBM) taking into account the energy lost during the photo-charge generation [30]. The theoretical values of Voc have been calculated from the following expression:

$Voc = |E_{HOMO} (Donor)| - |E_{LUMO} (Acceptor)| - 0.3$

The obtained Voc values of our studied compounds blended with the acceptors PCBM and C60-OMe, are shown in Table 3. The calculated Voc values range from (0.64 to 1.14 eV) /PBCM and from

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(1.44 to 1.96 eV) /C60-OMe. These values are sufficient for a possible efficient electron injection into LUMO of the acceptor.

In the other side, the table 3 shows that the differences (E_{LUMO} (Donor) - E_{LUMO} (acceptor)) of LUMO energy levels between the donors (studied molecules) and the acceptor (PCBM/C60-OMe) range from 0.64 to 1.14 eV/PCBM and from 1.44 to 1.94

eV/C60-OMe, these values are larger than 0 eV, which ensures efficient electron transfer from the donor to the acceptor.

Therefore, all the studied molecules can be used as BHJ because the electron injection process from the excited molecule to the conduction band of the acceptor (PCBM/C60-OMe).

**Table 3**: Energy Values of E_{HOMO}, E_{LUMO} and the Open Circuit Voltage Voc by eV.

Compounds	E_{HOMO} (eV)	E_{LUMO} (eV)	Voc (eV)/		α_i (eV)	
			C60-OMe	PCBM	C60-OMe	PCBM
M1	-5.14	-1.69	1.94	1.14	1.20	1.80
M2	-4.93	-1.57	1.73	0.93	1.33	2.13
M3	-4.64	-1.34	1.44	0.64	1.55	2.35
M4	-4.96	-1.89	1.76	0.96	1.01	1.81
M5	-4.85	-1.91	1.85	0.85	0.99	1.79
M6	-4.78	-1.96	1.58	0.78	0.93	1.73
M7	-4.86	-2.08	1.86	0.86	0.82	1.62
M8	-4.72	-2.21	1.52	0.72	0.69	1.49
C60-OMe	**-**	**-2.90**	-	-	-	-
PCBM	**-6.1**	**-3.7**	-	-	-	-

*α_i = E_{LUMO} (Donor) - E_{LUMO} (C60-OMe/PBCM); (The donor compounds are Mi; i=1…8).

3.4. Absorption properties

The absorption properties of organic material, is an important factor for the application as a photovoltaic material, and a good photovoltaic material must have widely and intense visible absorption characteristics. Starting with optimized geometry, the electronic absorption spectra of the studied molecules in vacuum are performed using TD-DFT/B3LYP/6-31G(d) calculations. The Table 4 presents the Data absorption spectra (Main transition states, their assignments, the corresponding wavelength and oscillator strength) for all compounds. The corresponding simulated UV–Vis absorption spectra of all studies compounds, presented as oscillator strength against wavelength are shown in Fig. 6. Excitation to the S1 state corresponds exclusively to the promotion of an electron from the HOMO to the LUMO orbital and is attributable to the π-π* transition. The absorption wavelengths arising from S0→S1 electronic transition increase progressively with the increasing of the electron donor strength substituents and with the decreasing of the band gap energies of the studied molecules. Table 5 and Fig. 6 show that there is a bathochromic shift when passing from Molecule M1 (379.74 nm) to Molecule M8 (533.60 nm) in the following order M1

→ M2 → M3 → M4 → M5 → M6 → M7 → M8. Moreover, M5 and M8 have an intense absorption (high oscillator strength) comparing with the other compounds. This effect is obviously due to the aromaticity and to the conjugated length in these compounds. Therefore, we remark that the spectrum obtained by TDDFT/B3LYP/6-31G(d) method is almost similar to that obtained experimentally for the compounds M1 (λexp = 355 nm) and M7 (λexp = 416 nm) [33]. We can conclude that the theoretical results obtained by TDDFT are in good agreement with the experimental ones.
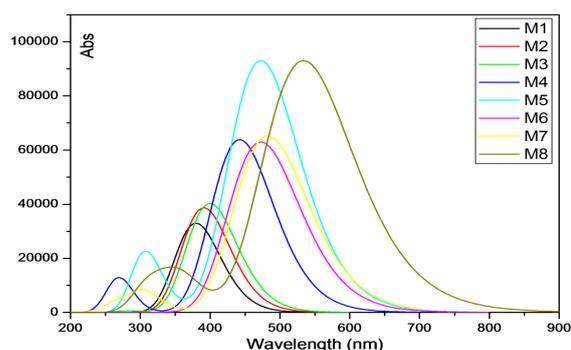
Figure 6: Simulated UV–visible optical absorption spectra of studied compounds with the calculated data at the TD/B3LYP/6-31G (d) level.

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Table 4. Data absorption spectra obtained by TD/DFT method for the studied compounds in the optimized geometries at B3LYP/6-31G(d).

Compounds	Electronic transitions	λabs (nm)	E (Cm⁻¹)	E_{ex} (eV)	O.S	MO/character (%)	λexp (nm)[33]
M1	$S_0 \rightarrow S_1$	**379.74**	**26333.37**	**3.26**	**0.81**	**HOMO → LUMO (100%)**	**355**
	$S_0 \rightarrow S_2$	299.62	33374.64	4.13	0.00	HOMO → LUMO+1 (65%)	
	$S_0 \rightarrow S_3$	272.74	36663.79	4.54	0.00	HOMO-1 → LUMO (50%)	
M2	$S_0 \rightarrow S_1$	**391.05**	**25571.98**	**3.17**	**0.95**	**HOMO → LUMO (100%)**	-
	$S_0 \rightarrow S_2$	306.83	32590.66	4.04	0.00	HOMO → LUMO+1 (58%)	
	$S_0 \rightarrow S_3$	278.87	35858.04	4.44	0.00	HOMO-1 → LUMO (53%)	
M3	$S_0 \rightarrow S_1$	**399.68**	**25019.49**	**3.10**	**0.99**	**HOMO → LUMO (100%)**	–
	$S_0 \rightarrow S_2$	315.12	31733.29	3.93	0.00	HOMO-1 → LUMO (61%)	
	$S_0 \rightarrow S_3$	291.17	34343.3	4.25	0.00	HOMO → LUMO+2 (96%)	
M4	$S_0 \rightarrow S_1$	**442.30**	**22608.68**	**2.80**	**1.57**	**HOMO → LUMO (100%)**	-
	$S_0 \rightarrow S_2$	357.49	27972.30	3.46	0.00	HOMO → LUMO+1 (65%)	
	$S_0 \rightarrow S_3$	322.2	31032.39	3.84	0.00	HOMO-1 → LUMO (65%)	
M5	$S_0 \rightarrow S_1$	**472.60**	**21159.29**	**2.62**	**2.29**	**HOMO → LUMO (100%)**	–
	$S_0 \rightarrow S_2$	386.50	25872.83	3.20	0.00	HOMO → LUMO+1 (56%)	
	$S_0 \rightarrow S_3$	358.73	27875.52	3.45	0.02	HOMO-1 → LUMO (57%)	
M6	$S_0 \rightarrow S_1$	**472.58**	**21160.10**	**2.62**	**1.55**	**HOMO → LUMO (100%)**	-
	$S_0 \rightarrow S_2$	388.58	25734.10	3.19	0.00	HOMO-1 → LUMO (62%)	
	$S_0 \rightarrow S_3$	340.08	29404.75	3.64	0.00	HOMO → LUMO+1 (62%)	
M7	$S_0 \rightarrow S_1$	**482.50**	**20725.36**	**2.57**	**1.61**	**HOMO → LUMO (100%)**	**416**
	$S_0 \rightarrow S_2$	397.17	25177.57	3.12	0.00	HOMO → LUMO+1 (56%)	
	$S_0 \rightarrow S_3$	351.88	28418.33	3.52	0.00	HOMO-1 → LUMO (57%)	
M8	$S_0 \rightarrow S_1$	**533.60**	**18740.42**	**2.32**	**2.29**	**HOMO → LUMO (100%)**	
	$S_0 \rightarrow S_2$	452.18	22115.06	2.74	0.00	HOMO → LUMO+1 (59%)	
	$S_0 \rightarrow S_3$	385.35	25950.26	3.21	0.00	HOMO-1 → LUMO (61%)	

4. CONCLUSION

In this work, the quantum chemical investigation on the geomectric and optoelectronic properties obtained by DFT/B3LYP/6-31G(d) and TDDFT/B3LYP/6-31G(d) calculations of various compounds based on terthiophene end-capped by several donor groups is performed in order to display the effect of substituents donor groups on the structural and opto-electronic properties of these compounds.

The modification of chemical structures by introduction of several electron donor groups can greatly modulate and improve the electronic and optical properties of the studied compounds. This modification destabilized the HOMO levels of M2-M8 compared with M1 (unsubstituted molecule: basic molecule).

The calculated band gap values by using DFT-B3LYP/631G(d) method are in the range of 2.51-3.44 eV and are decreasing in the following order: M1>M2>M3>M4>M5>M6>M7>M7>M8. The molecule M8 has the smallest band gap energy (2.51 eV). This is due to the effect of the strong electron-donor character of the thienylenevinylene unit and to the conjugated length.

The UV–Vis absorption properties have been obtained by using TDDFT/B3LYP/6-31G(d) method. The obtained absorption maximums are in the range from 379.74 to 533.60 nm.

The theoretical photovoltaic values of V_{oc} and α_i of the studied molecules range from 0.64 to 1.14 eV/PBCM, from 1.44 to 1.96 eV/C60-OM and from 0.64 to 1.14 eV/PCBM and 1.44 to 1.94 eV/C60-OMe respectively. These values are sufficient for a possible efficient electron injection from the excited molecule to the conduction band of PCBM/C60-OMe.

Finally, the obtained results demonstrate how the electronic properties can be tuned by the substituent with several donor groups and suggest these compounds as good candidates for optoelectronic applications such as BHJ in solar cells, in particularly the compound M8 (Eg = 2.51 eV, Voc = 0.72/PBCM and 1.52/C60-OMe, λabs = 533 nm/O.S = 2.32 eV).

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