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# Organic materials based on oxathiazole and thiophene for photovoltaic devices. Correlation structure/electronic properties

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## Abstract

In this work, the theoretical analysis on the geometries and electronic properties of conjugated compound based on thiophene and oxadiazole {TTTTT; TTTTT(CH3); OxTOxTOx(CH3) ;TTOxTT; TTOxTT(OMe); TTOxTT(CN) ;TTOxTT(F); TTOxTT(CH3)} .We presented a theoretical study by using DFT method at B3LYP level with 6-31G (d) basis set. The theoretical knowledge of the HOMO and LUMO energy levels of the components is basic in studying organic solar cells. So, the HOMO, LUMO, Gap energy and the photovoltaic properties of the studied compounds have been calculated. These properties suggest that these materials are a good candidate for organic solar cells.

*Keywords* : π-conjugated molecules, organic solar cells, thiophene, oxadiazole , DFT, low band-Gap, electronic properties, HOMO, LUMO.

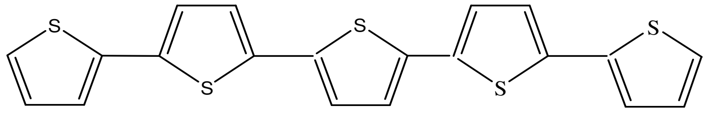
## Introduction

During the past decade, π-conjugated molecules based electronic materials have been extensively investigated as novel class of semi-conductors and are frequently studied because of their promising opto-electronic properties [1]. Due to their important specific properties, these new compounds had become the most promising materials for a range of industrial applications such as optoelectronic device technology [2], electroluminescent devices [3], field-effect transistors [4] and photovoltaic [5]. Therefore, designing and synthesizing conjugated molecules with interesting properties play a crucial role in technology at the same time it is important to understand the nature of the relationship between the molecular structure and the electronic properties to provide guidelines for the development of new materials. Many researchers have become interested in synthesizing short-chain compounds based on conjugated molecules because they are not amorphous and can be synthesized as well defined structures [6]. On the other hand and since the discovery of the ultra fast and ultra efficient photo induced electron transfer between π-conjugated systems and fullerene derivatives [7] considerable interest for hetero-junction solar cells based on interpenetrating networks of conjugated systems and C60 derivatives has been generated [8]. At the same time it is important to understand the nature of the relationship between the molecular structure and the electronic properties to provide guidelines for the development of new materials. Theoretical analysis of the electronic structure of conjugated systems can establish the relationships between molecular structure and electronic properties [9].

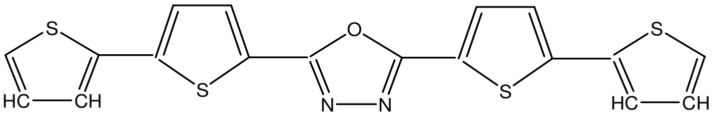
Theoretical studies on the electronic structures of π-conjugated compounds have given great contributions to the rationalization of the properties of known materials and to the properties prediction those of yet unknown ones. In this context, quantum chemical methods have been increasingly applied to predict the band gap of conjugated systems [10]. The HOMO and LUMO energy levels of the donor and of the acceptor components for photovoltaic devices are very important factors to determine whether the effective charge transfer will happen between donor and acceptor. The offset of band edges of the HOMO and LUMO levels will prove responsible for the improvement of all photovoltaic parameters of the organic solar cells.

In this work, the theoretical analysis on the geometries and electronic properties of conjugated compound based on thiophene and oxadiazole {OxTOxTOx($CH_3$); TTOxTT; TTOxTT(OMe); TTOxTT(CN); TTOxTT(F); TTOxTT($CH_3$)} is reported, as shown in figure 1,. These compounds were prepared by Toufik et al [11].

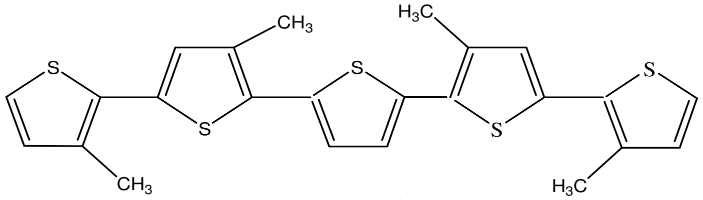
The theoretical ground-state geometry and electronic structure of the studied molecules were investigated by the DFT method at B3LYP level with 6-31G (d) basis set.



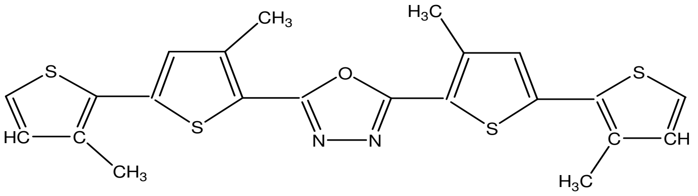
TTTTT



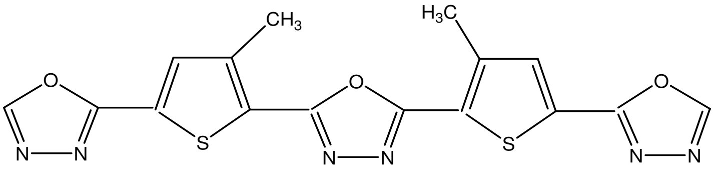
TTOxTT



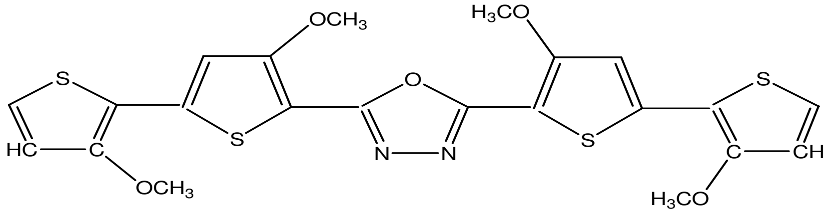
TTTTT($CH_3$)



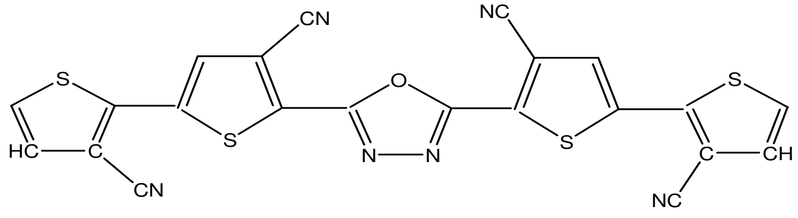
TTOxTTOx(CH3)



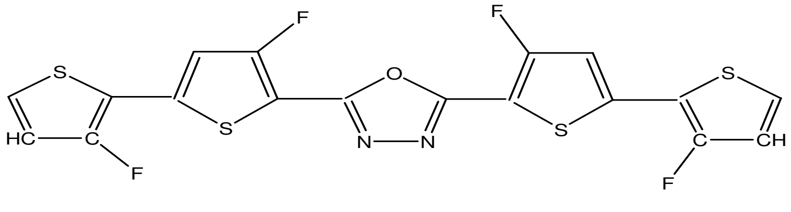
OxTOxTOx(CH3)



TTOxTTOx(OCH3)



TTOxTTOx(CN)



TTOxTTOx(F)

**Figure 1:** Chemical structure of studied compounds.

The theoretical knowledge of the HOMO and LUMO energy levels of the components is basic in studying organic solar cells so the HOMO, LUMO, Gap energy and Voc (open circuit voltage) of the studied compounds have been calculated and reported. The obtained properties suggest these materials as a good candidate for organic dye-sensitized solar cells.

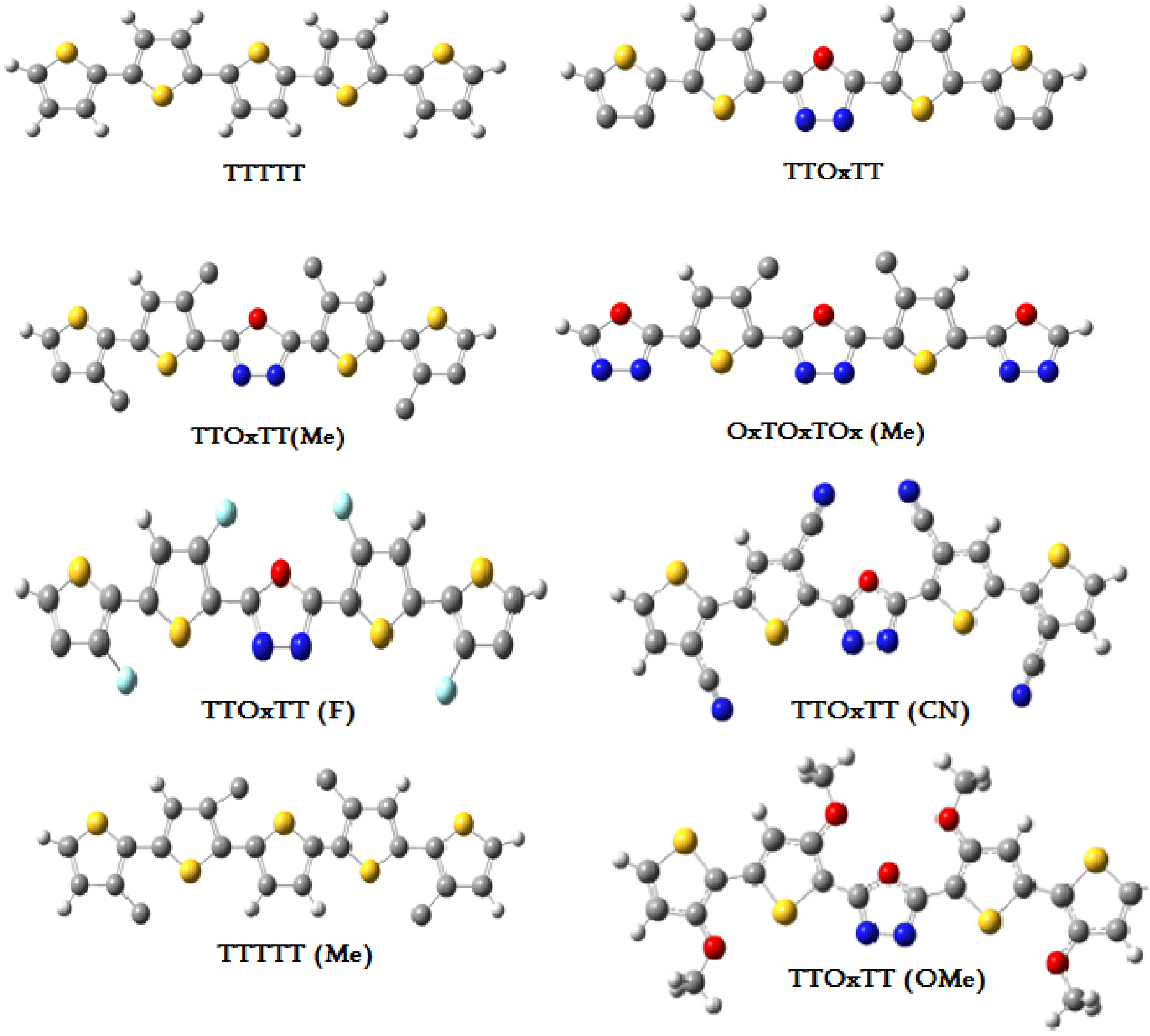
## 2. Materials and methods

DFT method of three-parameter compound of Becke (B3LYP) [12] was used in all the study of the neutral compound. The 6-31G (d) basis set was used for all calculations [13-14]. To obtain the charged structures, we start from the optimized structures of the neutral form. The calculations were carried out using the Gaussian 03 program [15]. The geometry structures of neutral and doped molecules were optimized under no constraint. We have also examined HOMO and LUMO levels and the corresponding energy gap evaluated as the difference between them.

## 3. Results and discussion

The chemical structure of all molecules studied is depicted in figure.1 and the optimized geometries of the studied molecules are plotted in figure.2. In order to determine the geometrical parameters, the molecules are fully optimized in their ground state using the 6-31G (d) basis set.

The results of the optimized structures (figure.2) for all studied compounds so that they have similar conformations (quasi planar conformation). We found that the modification of several groups attached to the Basic molecule does not change the geometric parameters.



TTTTT

TTOxTT

TTOxTT(Me)

OxTOxTOx (Me)

TTOxTT (F)

TTOxTT (CN)

TTTTT (Me)

TTOxTT (OMe)

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

**Table 1**: The HOMO energy ($E_{HOMO}$), LUMO energy ($E_{LUMO}$), and HOMO–LUMO energy gap ($E_{gap}$) in eV for ground state computed at the B3LYP/6-31G level of theories.

| Compounds | $E_{HOMO}$(eV) | $E_{LUMO}$(eV) | $E_{gap}$ |
|---|---|---|---|
| **TTTTT** | -4.860 | -2.080 | 2.78 |
| **TTOxTT** | -5.414 | -2.166 | 3.24 |
| **TTTTT (Me)** | -4.626 | -1.853 | 2.72 |
| **TTOxTT (Me)** | -5.125 | -1.980 | 3.14 |
| **OxTOxTOx (Me)** | -6.046 | -2.638 | 3.40 |
| **TTOxTT (OMe)** | -4.540 | -1.560 | 2.98 |
| **TTOxTT (CN)** | -6.246 | -3.255 | 2.99 |
| **TTOxTT (F)** | -5.452 | -2.212 | 3.23 |

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 HOMO and LUMO energies of studied compounds change significantly, the LUMOs for TTTTT; TTOxTT ; TTTTT(CH3); TTOxTT(CH3); OxTOxTOx(CH3); TTOxTT(OMe); TTOxTT(CN) ;TTOxTT(F) are located at -2.080; -2.166; -1.853; -1.980; -2.638; -1.560; -3.255 and -2.212 eV, respectively. The HOMOs for TTTTT; TTOxTT ; TTTTT(CH3); TTOxTT(CH3); OxTOxTOx(CH3); TTOxTT(OMe); TTOxTT(CN) ; TTOxTT(F) are located at -4.860; -5.414; -4.626; -5.125; -6.046; -4.540; -6.246 and -5.452 eV, respectively.
It can also be found that, the HOMO and LUMO energies of the studied compounds are slightly different. This implies that different structures play key roles on electronic properties and the effect of slight structural variations, especially the effect of the motifs branched to the molecule on the HOMO and LUMO energies is clearly seen. In addition, energy (Egap) of the studied molecules differs slightly from 2.72 eV to 3.40 eV. They are studied in the following order:

**OxTOxTOx(Me)>TTOxTT>TTOxTT(F)>TTOxTT(Me)>TTOxTT(CN)>TTOxTT(OMe)>TTTTT> TTTTT (Me)**

To evaluate the possibilities of electron transfer from the excited studied molecules to the conductive band of PCBM, the HOMO and LUMO levels were compared. Table 2 lists the calculated frontier orbital energies highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), the Egap energy of the studied molecules, the open circuit voltage Voc (eV) and The difference between both the energy levels LUMO of the donor and acceptor noted α [16].
On the other hand, concerning the study of Photovoltaic Properties and knowing that generally, the most efficient material solar cells are based on the bulk hetero-junction structure of the blend of π-conjugated molecule or polymer donors and fullerene derivative acceptors [17-18]. Here, we studied and discuss the photovoltaic properties of the compounds TTTTT; TTOxTT ; TTTTT(CH3); TTOxTT(CH3); OxTOxTOx(CH3); TTOxTT(OMe); TTOxTT(CN) ;TTOxTT(F) as donor blended with [6.6]-phenyl-C61-butyric acid methyl ester (PCBM), which is 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. Figure 4 shows detailed data of absolute energy of the frontier orbitals for the studied compounds and PCBM derivatives. It is deduced that the nature of donor or acceptor pushes up/down the HOMO/LUMO energies in agreement with their electron character. To evaluate the possibilities of electron transfer from the excited studied molecules to the conductive band of PCBM, the HOMO and LUMO levels were compared.
Finally, and from the above analysis, we know that the LUMO energy levels of the studied molecules is much higher than that of the ITO conduction band edge (-4.7 eV).Thus, the studied molecules TTTTT; OxTOxTOx(CH3) ;TTOxTT; TTOxTT(OMe) ;TTOxTT(CN) ;TTOxTT(F) and TTOxTT(CH3) have a strong ability to inject electrons into ITO electrodes. The experiment phenomenon is quite consistent with previous literature [19], this latter reported that the increase of the HOMO levels may suggest a negative effect on organic solar cell performance due to the broader gap between the HOMO level of the organic molecules and the HOMO level of several acceptor PCBM. ($C_{60}$, $C_{70}$, $C_{76}$, $C_{78}$-$C_{2V}$, $C_{78}$-$D_3$, $C_{84}$-$D_3$, $C_{84}$-$D_2$, $C_{84}$-$D_{2d}$) (Figure 3).

**Table 2**: Energy Values of $E_{LUMO}$ (eV), $E_{HOMO}$ (eV), $E_{gap}$ (eV), α and the Open Circuit Voltage Voc (eV) of the Studied Molecules obtained by B3LYP/6-31G (d).

| | | | | **PCBM $C_{60}$ (A)** | | **PCBM $C_{60}$** | | **PCBM $C_{70}$** | | **PCBM $C_{76}$** | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Compounds** | **$E_{HOMO}$ (eV)** | **$E_{LUMO}$ (eV)** | **$E_{gap}$ (eV)** | **$V_{oc}$ (eV)** | **α (eV)** | **$V_{oc}$ (eV)** | **α (eV)** | **$V_{oc}$ (eV)** | **α (eV)** | **$V_{oc}$ (eV)** | **α (eV)** |
| **TTTTT** | -4.860 | -2,080 | 2.78 | 0.860 | 1.620 | 1.09 | 1.39 | 1.02 | 1.46 | 0.770 | 1.710 |
| **TTOxTT** | -5.414 | -2,166 | 3.24 | 1.414 | 1.534 | 1.644 | 1.304 | 1.574 | 1.374 | 1.324 | 1.624 |
| **TTTTT (Me)** | -4.626 | -1,853 | 2.72 | 0.626 | 1.847 | 0.856 | 1.617 | 0.786 | 1.687 | 0.536 | 1.937 |
| **TTOxTT (Me)** | -5.125 | -1,980 | 3.14 | 1.125 | 1.720 | 1.355 | 1.49 | 1.285 | 1.56 | 1.035 | 1.810 |
| **OxTOxTOx (Me)** | -6.046 | -2,638 | 3.40 | 2.046 | 1.062 | 2.276 | 0.832 | 2.206 | 0.902 | 1.956 | 1.152 |
| **TTOxTT (OMe)** | -4.540 | -1,560 | 2.98 | 0.540 | 2.140 | 0.77 | 1.91 | 0.7 | 1.98 | 0.450 | 2.230 |
| **TTOxTT (CN)** | -6.246 | -3,255 | 2.99 | 2.246 | 0.445 | 2.476 | 0.215 | 2.406 | 0.285 | 2.156 | 0.535 |
| **TTOxTT (F)** | -5.452 | -2,212 | 3.23 | 1.452 | 1.488 | 1.682 | 1.258 | 1.612 | 1.328 | 1.362 | 1.578 |
| **PCBM $C_{60}$ (A)** | -6.1 | -3,700 | | | | | | | | | |
| **PCBM $C_{60}$** | - | -3,470 | | | | | | | | | |
| **PCBM $C_{70}$** | - | -3,540 | | | | | | | | | |
| **PCBM $C_{76}$** | - | -3,790 | | | | | | | | | |

| | | | | **PCBM $C_{78-C2V}$** | | **PCBM $C_{78-D3}$** | | **PCBM $C_{84-D2}$** | | **PCBM $C_{84-D2d}$** | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Compounds** | **$E_{HOMO}$ (eV)** | **$E_{LUMO}$ (eV)** | **$E_{gap}$ (eV)** | **$V_{oc}$ (eV)** | **α (eV)** | **$V_{oc}$ (eV)** | **α (eV)** | **$V_{oc}$ (eV)** | **α (eV)** | **$V_{oc}$ (eV)** | **α (eV)** |
| **TTTTT** | -4.860 | -2.080 | 2.78 | 0.620 | 1.860 | 0.560 | 1.920 | 0.580 | 1.900 | 0.610 | 1.870 |
| **TTOxTT** | -5.414 | -2.166 | 3.24 | 1.174 | 1.774 | 1.114 | 1.834 | 1.134 | 1.814 | 1.164 | 1.784 |
| **TTTTT (Me)** | -4.626 | -1.853 | 2.72 | 0.386 | 2.087 | 0.326 | 2.147 | 0.346 | 2.127 | 0.376 | 2.097 |
| **TTOxTT (Me)** | -5.125 | -1.980 | 3.14 | 0.885 | 1.960 | 0.825 | 2.020 | 0.845 | 2.000 | 0.875 | 1.970 |
| **OxTOxTOx (Me)** | -6.046 | -2.638 | 3.4 | 1.806 | 1.302 | 1.746 | 1.362 | 1.766 | 1.342 | 1.796 | 1.312 |
| **TTOxTT (OMe)** | -4.540 | -1.560 | 2.98 | 0.300 | 2.380 | 0.240 | 2.440 | 0.260 | 2.420 | 0.290 | 2.390 |
| **TTOxTT (CN)** | -6.246 | -3.255 | 2.99 | 2.006 | 0.685 | 1.946 | 0.745 | 1.966 | 0.725 | 1.996 | 0.695 |
| **TTOxTT (F)** | -5.452 | -2.212 | 3.23 | 1.212 | 1.728 | 1.152 | 1.788 | 1.172 | 1.768 | 1.202 | 1.738 |
| **PCBM $C_{78- C2V}$** | - | -3.94 | | | | | | | | | |
| **PCBM $C_{78-D3}$** | - | -4.00 | | | | | | | | | |
| **PCBM $C_{84-D2}$** | - | -3.98 | | | | | | | | | |
| **PCBM $C_{84-D2d}$** | - | - 3.95 | | | | | | | | | |

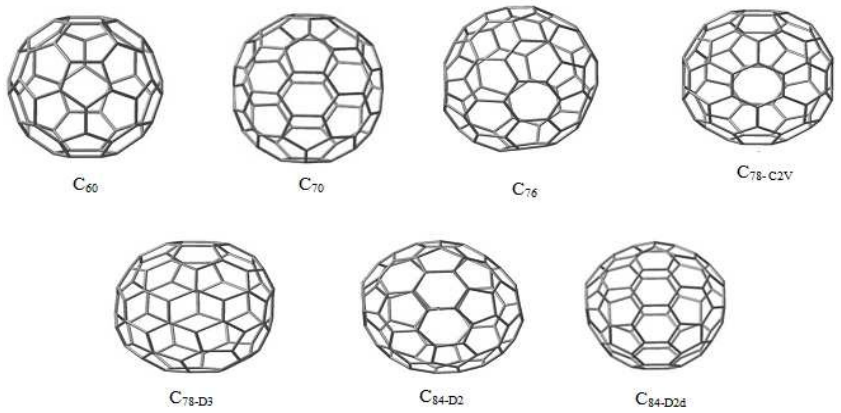


**Figure 3:** Structure of the investigated fullerenes.

It is known that the architecture of photoactive layer is one of the principle factors of efficiencies of solar cells. The most efficient technique to generate free charge carriers is bulk heterojunction where the π-conjugated compounds donors are blended with fullerene derivatives us acceptor [20]. In our study, PCBM and derivatives ($C_{60}$,$C_{70}$,$C_{76}$, $C_{78}$-$C_{2V}$, $C_{78}$-$D_3$, $C_{84}$-$D_2$, $C_{84}$-$D_{2d}$) were included for comparison purposes.

As shown in table 2, both HOMO and LUMO levels of the studied molecules agree well with the requirement for an efficient photosentizer. It should be noted that the LUMO levels of the studied compounds are higher than that of PCBM derivatives which varies in literature from -4.0 to -3.47 eV ($C_{60}$ (-3.47 eV), $C_{70}$ (-3.54), $C_{76}$ (-3.79), $C_{78}$-$C_{2V}$ (-3.94), $C_{78}$-$D_3$ (-4.0), $C_{84}$-$_{D2}$ (-3.98), $C_{84}$-$_{D2d}$ (-3.95) [21].

The bulk-heterojunction (BHJ) cells combine the advantages of easier fabrication and higher conversion efficiency due to the considerably extended D/A interface. The BHJ solar cells have been essentially based on the use of soluble π-conjugated polymers as donor material, owing to a useful combination of optical and charge-transport properties. However, besides the limit imposed to the maximum conversion efficiency by its intrinsic electronic properties, P3HT and more generally polymers pose several problems related to the control of their structure, molecular weight, polydispersity, and purification [22].

To evaluate the possibilities of electron transfer from the studied molecules to the conductive band of the proposed acceptors, the HOMO and LUMO levels are compared. 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. The maximum open circuit voltage ($V_{oc}$) of the BHJ solar cell is related to the difference between the highest occupied molecular orbital (HOMO) of the donor (our studied molecules) and the LUMO of the electron acceptor (PCBM derivatives in our case), taking into account the energy lost during the photo-charge generation [23]. The theoretical values of open-circuit voltage $V_{oc}$ have been calculated from the following expression:

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

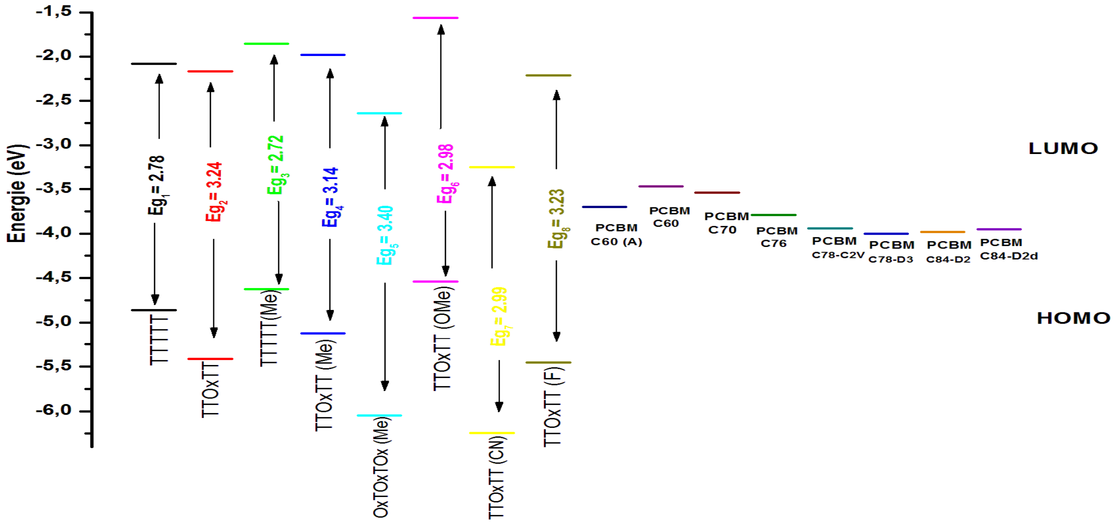


**Figure 4:** shows detailed data of energy of the frontier orbitals for studying compounds with PCBM and its derivatives.

The obtained values of Voc of the studied molecules (TTTTT; TTOxTT; TTTTT (Me); TTOxTT (Me); OxTOxTOx (Me); TTOxTT (OMe); TTOxTT (CN); TTOxTT (F)) calculated according to the expression range respectively from (0,86eV.1,414eV; 0,626 eV; 1,125eV; 2,046eV; 0,540eV; 2,246eV; 1,452eV ) for PCBM C60(A); (1,09eV; 1,644eV 0,856eV; 1,355eV; 2,27eV; 0,77eV; 2,476eV; 1,682eV) for PCBMC60; (1,106eV; 1,574 eV, 0,786eV; 1,285eV ;2,206eV; 0,7eV; 2,406eV;1,612eV) for PCBMC70;(0,77eV; 1,324eV;0,536eV;1,035eV; 1,956eV; 0;45eV; 2,156eV; 1,362eV) for PCBM C76 ;(0,62eV; 1,174eV;0,386eV;0,885eV; 1,806eV; 0,3eV; 2,006eV; 1,212eV) for PCBM C78 C2V; (0,56eV; 1,114eV; 0,326eV; 0,825eV;1,746eV; 0,24eV;1,946eV;1,152eV) for PCBM C78-D3; (0,58eV; 1,134eV; 0,346eV;0,845eV; 1,766eV; 0,26eV; 1,966eV; 1,172eV) for PCBM C78-D2; (0.610eV; 1.164eV; 0.376eV; 0.875eV; 1.796eV; 0.290eV; 1.996eV; 1.202eV) for PCBM C78-D2 (see Table 2). These values are sufficient for a possible efficient electron injection.

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 PCBM derivatives and the subsequent regeneration is possible in an organic solar cell. We noted that the best values of Voc are indicated for the studied compounds) blended with C60 (2,476eV) and C70 (2,406eV), and the higher value are given for molecule TTOxTT(CN) blended with C60 (2,476eV).

## Conclusion

This study is a theoretical analysis of the geometries and electronic properties of the compounds based on oxathiazol and tiophene which displays the effect of substituted groups on the structural and optoelectronic properties of these materials and leads to the possibility to suggest these materials for organic solar cells application. The concluding remarks are:

* The results of the optimized structures for the studied compounds show that they have similar conformations (quasi planar conformation). We found that the modification of the groups does not change the geometric parameters.

*.The calculated frontier orbital energies HOMO and LUMO and energy gaps showed that the energy gaps of the studied molecules differ slightly from 3,14eV to 2,72eV depending on the different structures.

* The best values of Voc are indicated for the studied compounds blended with C60 (2,476eV) and C70 (2,406eV), and the higher value are given for molecule TTOxTT(CN) blended with C60.

* All the studied molecules can be used as sensitizers because the electron injection process from the excitedmolecule to the conduction band of PCBM and derivatives and the subsequent regeneration are feasible in theorganic sensitized solar cell.

* This calculation procedure can be used as a model system for understanding the relationships between electronic properties and molecular structure and also can be employed to explore their suitability in electroluminescent devices and in related applications. Presumably, the procedures of theoretical calculations can be employed to predict and assume the electronic properties on yet prepared and efficiency proved the other materials, and further to design new materials for organic solar cells.

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