



## Theoretical study of the effect of substitution with alternating donor and acceptor groups on the optoelectronic and photovoltaic properties of some oligomers containing thiophene and phenylene

S. Boussaidi<sup>1,2</sup>, Y. Alaoui<sup>2,3</sup>, A. Eddiouane<sup>1,2</sup>, A. Fitri<sup>3</sup>, A. Benjelloun Touimi<sup>3</sup>,  
H. Zgou<sup>2\*</sup>, H. Chaib<sup>2</sup>, M. Bouachrine<sup>4</sup>, M. Hamidi<sup>5</sup>, T. Ben Hadda<sup>6</sup>

<sup>1</sup>Ibn Zohr University, Faculty of Sciences, B.P. 8106, 80090 Agadir, Morocco.

<sup>2</sup>Ibn Zohr University, Polydisciplinary Faculty, B.P. 638, 45000 Ouarzazate, Morocco.

<sup>3</sup>Sidi Mohamed Ben Abdallah University, LIMME, Faculty of Sciences Dhar Elmahraz, P.O. 1796 Fez-Atlas 30003, Fez, Morocco.

<sup>4</sup>Moulay Ismail University, MEM, High School of Technology (ESTM), P.O Box 3103 Toulal, 50040 Meknes, Morocco.

<sup>5</sup>Moulay Ismail University, Faculty of Sciences and Technology, P.O Box 509 Boutalamine, 52000 Errachidia, Morocco.

<sup>6</sup>Mohammed I<sup>st</sup> University, LCM Faculty of Sciences, BV Mohamed VI, P.O Box 717, 60000 Oujda, Morocco.

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### Abstract

In this paper, we carried out a theoretical investigation on several conjugated oligomers based on thiophene and phenylene without and with lateral acceptor and donor substituents. The aim of this work is to study the effect of these lateral groups on the structural, optoelectronic and photovoltaic properties of all oligomers. The theoretical ground-state geometries and electronic structures of the studied molecules were obtained using the density functional theory (DFT) method at B3LYP level with 6-31G(d) basis set. The optoelectronic properties (HOMO, LUMO, Egap...) were determined from the fully optimized structures. The absorption properties ( $\lambda_{\max}$ , E<sub>tr</sub>, OS) of these molecules are obtained by TD-B3LYP/6-31G(d) method. All calculations were realized by Gaussian 09 program supported by GaussView 5.0 .8 interface. The results of these investigations indicate how the photovoltaic properties can be tuned by introducing the electron-donating and electron-withdrawing groups on oligomer backbone. We suggest that these organic materials are good candidates for photovoltaic applications.

**Keywords:** Conjugated, Materials, Organic, Thiophene, Phenylene, Photovoltaic properties, DFT, TD.

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\*Corresponding author.

E-mail address: [zgouhsaine@gmail.com](mailto:zgouhsaine@gmail.com)

## 1. Introduction

Over the last 20 years [1], organic solar cells have caught the attention of many researcher groups due to their ability to afford high operating speeds, large device densities, low cost, and large area flexible circuits [2].

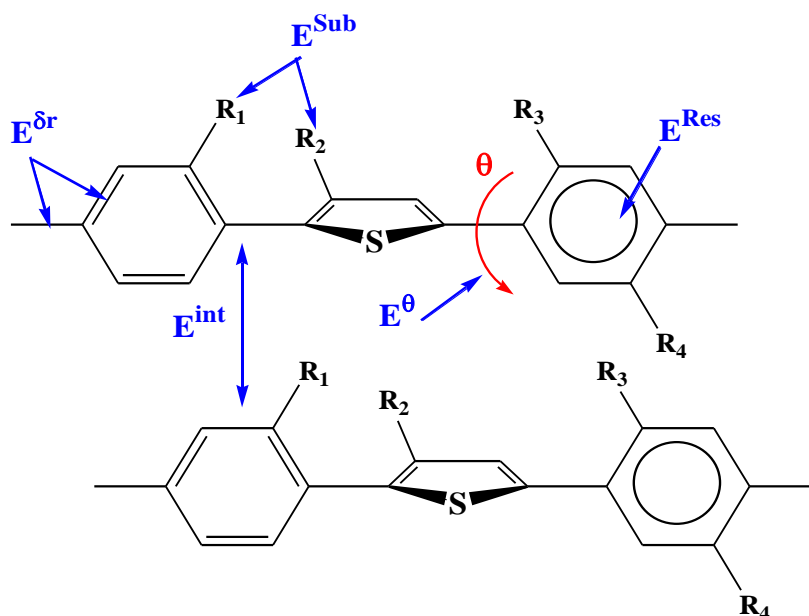
The bulk heterojunction (BHJ) organic semi-conductors have become one of the most successful device structures developed in the field to date. Following this development, recent years have seen a dramatic improvement in the efficiency of organic solar cells from 1% to 12% [3].

In principle, the strategies used to improve BHJ solar cell efficiency include (i) reducing the bandgap of organic material and (ii) lowering its HOMO, which increases the open-circuit voltage ( $V_{oc}$ ).

As mentioned in the literature, the bandgap of polyaromatic  $\pi$ -conjugated systems is determined by five contributions i.e. the energy related to bond length alternation,  $E^{\delta r}$ , the mean deviation from planarity  $E^{\theta}$ , the aromatic resonance energy of the cycle  $E^{Res}$ , the inductive or mesomeric electronic effects of eventual substitution  $E^{Sub}$ , and the intermolecular or inter-chain coupling in the solid state  $E^{int}$  [4].

$$E_g = E^{\delta r} + E^{\theta} + E^{Res} + E^{Sub} + E^{int}$$

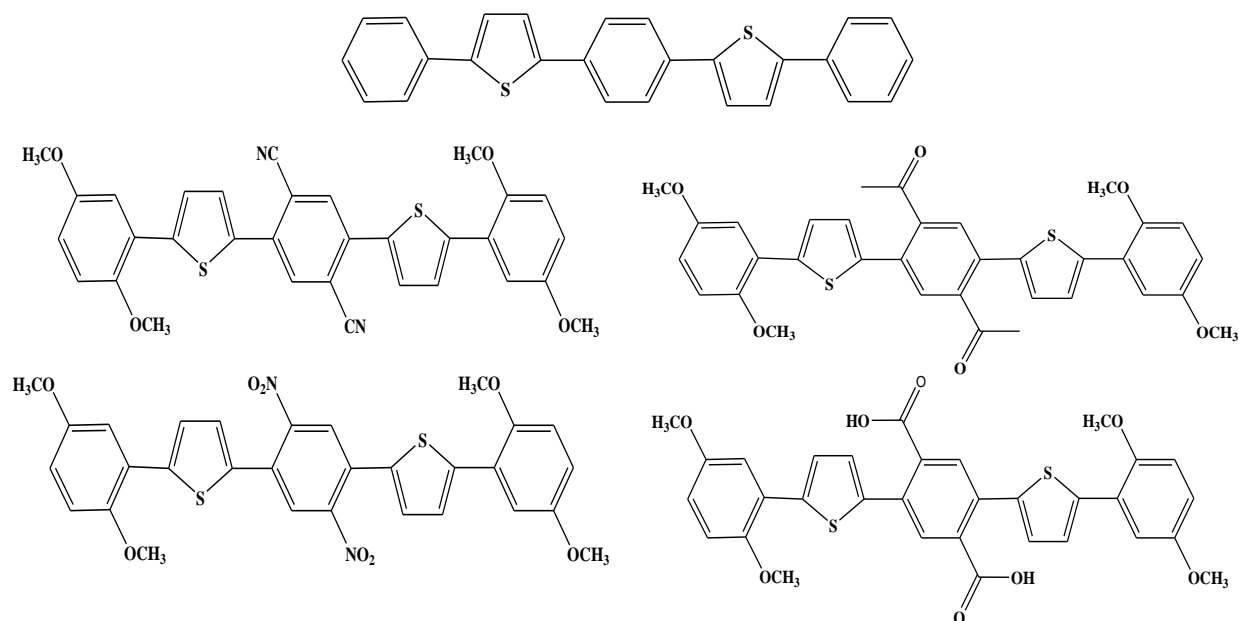
They are presented in the following Fig. 1:



**Figure 1:** Various energy contributions in the gap

Therefore, we attempted to examine the parameters  $E^{sub}$ . This latter is influenced by the nature of substituents, which may be a donor or acceptor. Introducing these substituents can, respectively, raise the HOMO level and decrease the LUMO level of the organic material.

In this article, we have used the density functional theory (DFT) calculations in order to study the effect of lateral groups on the geometrical, optoelectronic and photovoltaic properties of some oligomers based on thiophene and phenylene. The studied oligomers are shown in the Fig. 2.



**Figure 2:** The studied chemical structures.

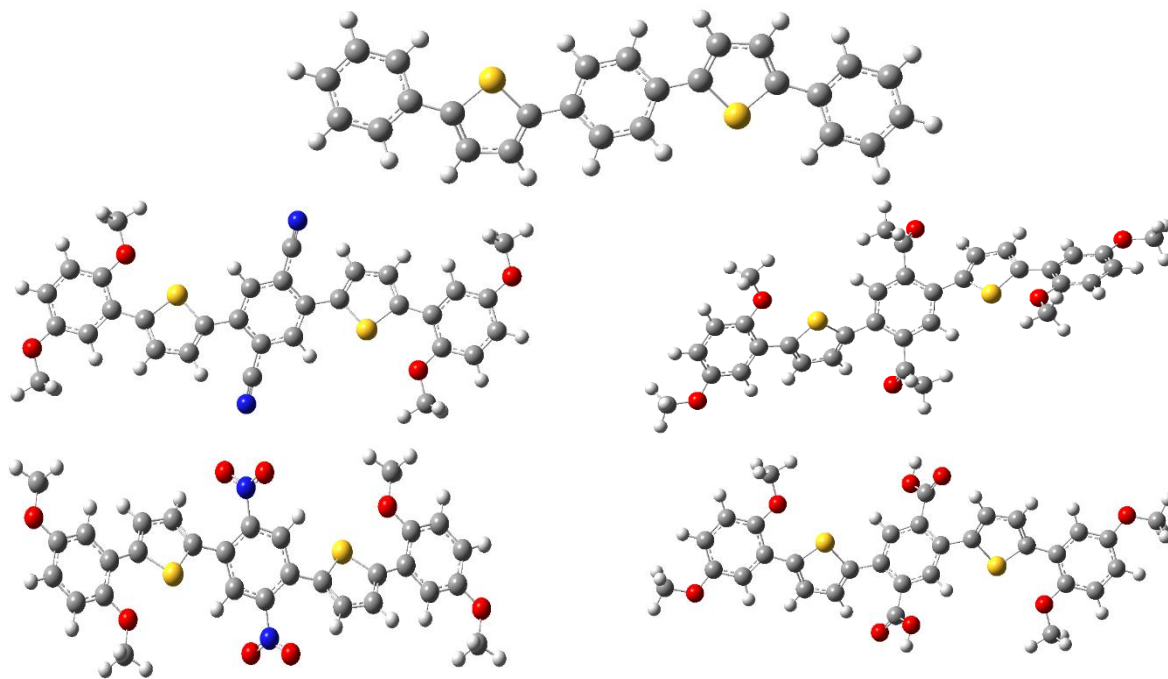
## 2. Computational methodology

Quantum calculations were carried out using the ‘Gaussian 09’ program [5]. The geometries of all oligomers were optimized using the DFT-B3LYP level which stands for Becke three parameters and Lee-Yang-Parr functional [6]. The 6-31G\* [7] basis set was used for all atoms. The geometrical structures of the neutral molecules were optimized under no constraint. The HOMO, LUMO and the gap energies were deduced from the stable structures, where the energy gap is the difference between LUMO and HOMO levels. The ground-state energies and oscillator strengths were computed using TD-DFT/B3LYP calculations on the fully optimized geometries. These calculation methods have been successfully applied to other conjugated polymers [8-11].

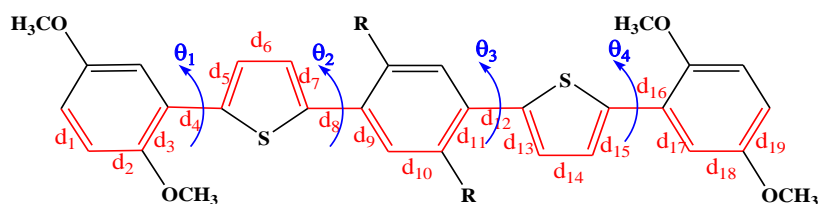
## 3. Results and discussion

### 3.1. Structural properties

The optimized ground state geometries of the oligomers obtained at the B3LYP/6-31G(d) level are given in Fig. 3. The calculated inter-atomic bond lengths ( $d_i$ ) and dihedral angles ( $\Theta_i$ ) are exhibited in Fig 4, and their optimized values are summarized in Table 2 and Table 3 respectively.



**Figure 3:** Optimized geometries of the studied oligomers



**Figure 4:** The labeled bond lengths and dihedral angles.

PTPTP is the unsubstituted oligomer and is used here as a reference [8]; For the unsubstituted oligomer (PTPTP), the B3LYP/6-31G(d) calculations predict that the dihedral angles are  $\theta_1=26.5^\circ$ ,  $\theta_2=23.5^\circ$ ,  $\theta_3=23.5^\circ$ , and  $\theta_4=26.5^\circ$ . The effect of substituents (donor and acceptor ones) grafted on phenylene rings exhibited clearly in structural properties. The values of dihedral angles  $\theta_1$  and  $\theta_4$  reduced nearly to  $16^\circ$  for oligomers 1 and 2 and to  $17^\circ$  for oligomers 3 and 4. Moreover the acceptor substituents grafted on the phenylene localized amidst of oligomers raise the dihedral angle  $\theta_2$  and  $\theta_3$  in comparison with the unsubstituted oligomer PTPTP.

The interatomic distances ( $d_i$ ) take small values for  $d_i=1, 5, 7, 9, 7, 11, 13, 15, 17, 19$  and high values for  $d_i=2, 4, 6, 8, 10, 12, 14, 16$ . The inter-ring distances ( $d_i=4, 8, 12, 16$ ) take the highest value which is near of the  $1.46 \text{ \AA}$ . this implies that these bonds are sometimes simple and sometimes double thus promoting a good combination and delocalization of electrons  $\pi$ .

**Table 1:** Bond-length ( $\text{\AA}$ ) values of the studied oligomers.

DISTANCES	PTPTP	Oligomer 1 COCH <sub>3</sub>	Oligomer 2 CN	Oligomer 3 COOH	Oligomer 4 NO <sub>2</sub>
<b>d<sub>1</sub></b>	1.386	1.395	1.399	1.395	1.389
<b>d<sub>2</sub></b>	1.406	1.398	1.393	1.398	1.340
<b>d<sub>3</sub></b>	1.420	1.400	1.411	1.400	1.413
<b>d<sub>4</sub></b>	1.469	1.470	1.468	1.469	1.468
<b>d<sub>5</sub></b>	1.381	1.382	1.384	1.382	1.384
<b>d<sub>6</sub></b>	1.414	1.415	1.412	1.414	1.413
<b>d<sub>7</sub></b>	1.380	1.378	1.380	1.378	1.379
<b>d<sub>8</sub></b>	1.465	1.473	1.461	1.473	1.470
<b>d<sub>9</sub></b>	1.402	1.418	1.422	1.405	1.406
<b>d<sub>10</sub></b>	1.399	1.397	1.399	1.398	1.389
<b>d<sub>11</sub></b>	1.421	1.406	1.403	1.419	1.414
<b>d<sub>12</sub></b>	1.465	1.473	1.461	1.473	1.470
<b>d<sub>13</sub></b>	1.380	1.377	1.380	1.378	1.379
<b>d<sub>14</sub></b>	1.414	1.416	1.412	1.414	1.413
<b>d<sub>15</sub></b>	1.381	1.382	1.384	1.382	1.383
<b>d<sub>16</sub></b>	1.469	1.470	1.468	1.469	1.468
<b>d<sub>17</sub></b>	1.420	1.400	1.411	1.420	1.410
<b>d<sub>18</sub></b>	1.406	1.398	1.393	1.393	1.394
<b>d<sub>19</sub></b>	1.386	1.395	1.399	1.399	1.399

**Table 2:** Dihedral angle ( $^{\circ}$ ) values of the studied compounds

Oligomers	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$
<b>PTPTP</b>	26.5	23.5	23.5	26.5
<b>Oligomer 1(COCH<sub>3</sub>)</b>	16.22	49.09	47.03	16.59
<b>Oligomer 2 (CN)</b>	16.44	31.18	31.18	16.40
<b>Oligomer 3 (COOH)</b>	17.04	49.82	49.82	17.04
<b>Oligomer 4 (NO<sub>2</sub>)</b>	17.44	53.05	53.07	17.49

### 3.2. Electronic properties :

The electronic properties depend essentially on the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) energy levels, and the electron hole mobility. In order to have the electronic properties study of the all oligomers, we calculated HOMO and LUMO energy levels and the band gap energies of the studied molecules, the values of these energies are presented in the [Table 3](#).

**Table 3 :** The  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and  $E_{\text{gap}}$  energies of studied oligomers.

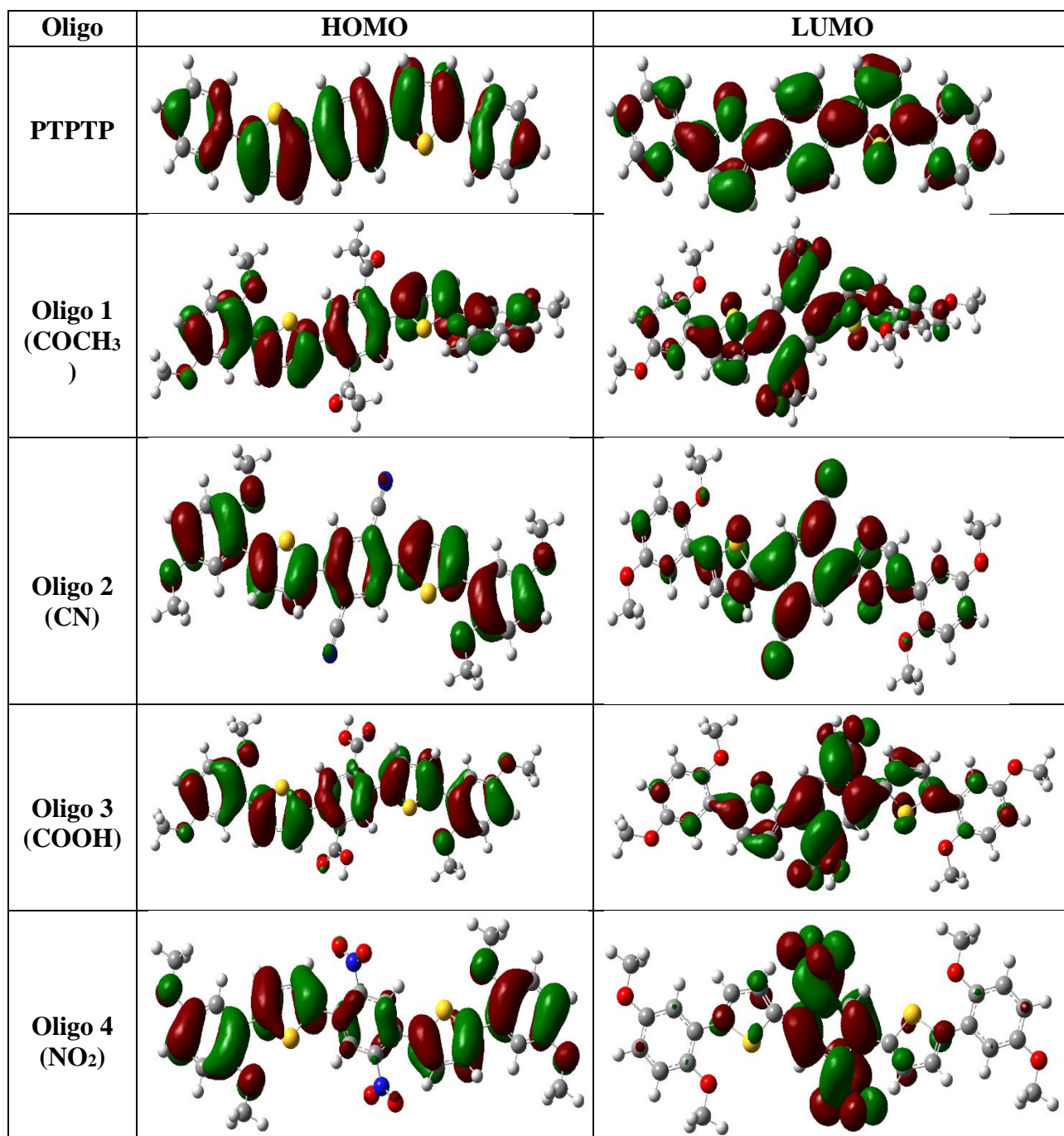
Oligomers	$E_{\text{HOMO}}$ (eV)	$E_{\text{LUMO}}$ (eV)	$E_{\text{gap}}$ (eV)
<b>PTPTP</b>	-5.16	-1.69	3.47
<b>Oligomer 1 (COCH<sub>3</sub>)</b>	-5.06	-1.60	3.46
<b>Oligomer 2 (CN)</b>	-5.22	-2.33	2.89
<b>Oligomer 3 (COOH)</b>	-4.99	-2.17	2.82
<b>Oligomer 4 (NO<sub>2</sub>)</b>	-5.30	-2.73	2.57

The band gap energy is evaluated by the difference between the LUMO and HOMO levels. Table 3 shows that the energy  $E_{\text{gap}}$  of the studied oligomers (i=1-5) are 3.47 eV, 3.47 eV, 2.89 eV, 2.82 eV and 2.57 eV respectively. The  $E_{\text{g}}$  is much affected by the change of acceptor substituents. These results can be explained by the electron-withdrawing power of the acceptor groups (COCH<sub>3</sub>, CN, COOH and NO<sub>2</sub>) and electron-donating of the donor groups (OCH<sub>3</sub>) introduced in each oligomer chains. We have plotted in Fig. 5 the contour plots of the HOMO and LUMO orbitals of all oligomers in their completely optimized conformation B3LYP/6-31G(d).

Generally we observe the electronic density in the HOMO it distributes evenly along the oligomer chains. In contrast, the LUMO have an obvious change between the unsubstituted oligomer and the others; the moving of the electronic density to the center of the chain of the substituted oligomers owing to attractor effect of the acceptor substituents. Also the LUMO orbitals became more concentrated around the acceptor substituents with increasing of its acceptor mesomeric -M effect in the following order COCH<sub>3</sub><CN<COOH<NO<sub>2</sub>. These results explain the decreasing of the band energy  $E_{\text{g}}$  Oligo (COCH<sub>3</sub>)< Oligo (CN)< Oligo (COOH)< Oligo (NO<sub>2</sub>).

### 3.3. Optical properties

The Table 4 shows the vertical excitation energy  $E_{\text{tr}}$ (eV), theoretical absorption  $\lambda_{\text{max}}$ (nm), oscillator strength (O.S) and molecular orbital character (MO/character) along with the main excitation configuration of all the molecules. These values are calculated by the TD/DFT/6-31G(d) method starting with the optimized geometries obtained by B3LYP/6-31G(d) level. The obtained results demonstrate that the lowest singlet electronic excitation is characterized as a typical  $\pi$ - $\pi^*$  transition with a significant intramolecular charge transfer.

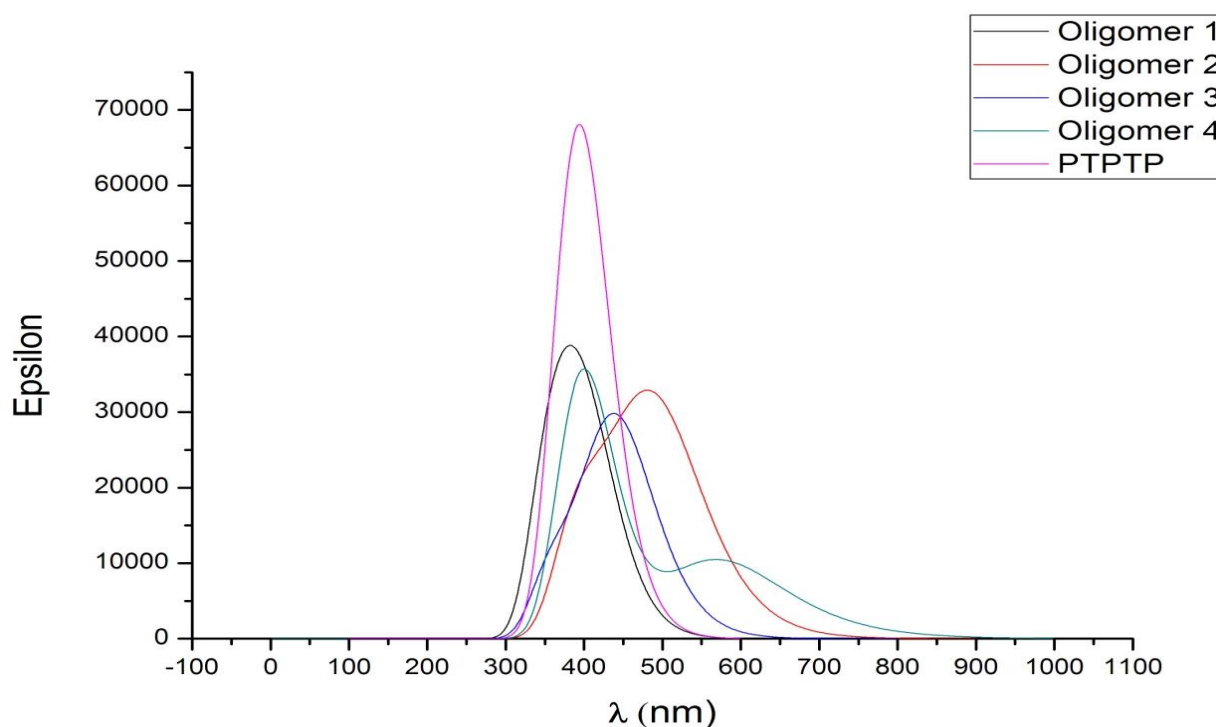


**Figure 5:** Contour plots of the molecular frontier orbitals of the studied molecules obtained by B3LYP/6-31G(d).

It is seen that the oligomer with NO<sub>2</sub> in the middle chains has the highest  $\lambda_{\max}$  among the donor-acceptor-substituted oligomers. Moreover, all oligomers having acceptor and donor groups have larger  $\lambda_{\max}$  compared with the unsubstituted one. These results confirm those electronic ones obtained in the last paragraph. The [Figure 6](#) shows the simulated absorption spectra of all the studied compounds.

**Table 4:** Calculated wavelength  $\lambda$ , Transition Energies and Oscillator Strengths (f) of all oligomers obtained by TD/B3LYP/6-31G(d) method.

Oligomer	$\lambda_{ab}(\text{nm})$	$E_{tr}(\text{eV})$	OS	CI coefficients
PTPTP	394.19	3.14	1.6811	H→L ( 0.70478)
	331.40	3.74	0.0000	H-1→L ( 0.52308), H→L +1(0.46651)
	308.98	4.01	0.0000	H-1→L ( -0.46922), H→L +1(0.52334)
Oligomer 1 COCH <sub>3</sub>	404.35	3.06	0.6445	H→L (0.69258), H→L+1(0.10234)
	367.69	3.37	0.0129	H-1→L( 0.68478)
	357.85	3.46	0.5667	H→L ( -0.10937), H→L+1(0.68086)
Oligomer 2 CN	490.96	2.52	0.7521	H→L (0.70127 )
	440.30	2.81	0.0000	H-1→L (0.70095)
	397.90	3.11	0.4497	H-2→L ( -0.14519).H→L+1 (0.67919)
Oligomer 3 COOH	441.70	2.81	0.7094	H→L (0.69973 )
	399.15	3.10	0.0000	H-1→L(0.69594 )
	362.66	3.42	0.2595	H-2→L ( -0.37080),H→L+1 (0.58306)
Oligomer 4 NO <sub>2</sub>	573.36	2.16	0.2543	H→L (0.70199)
	522.29	2.37	0.0000	H-1→L(0.70213)
	430.07	2.88	0.0234	H-2→L ( 0.69577)
	422.98	2.93	0.0000	H-2→L +1( -0.10786),H→L +1( 0.68841)
	403.66	3.07	0.0000	H-3→L( 0.68766), H→L +1( -0.10168)
	399.66	3.10	0.8637	H-1→L +1( -0.12828),H→L+2( 0.68282)

**Figure 6:** Calculated UV-vis spectra of the studied oligomers obtained by TD-DFT/B3LYP/6-31G(d)

### 3.4. Photovoltaic properties

In general, the most efficient organic solar cells are based on the bulk heterojunction (BHJ) structure of the blend of organic material donors and fullerene derivative acceptors (PC<sub>60</sub>BM) [12,13].

The introduction of electron-donating and electron-withdrawing groups represents the most important way to tune the HOMO and LUMO energy levels of a conjugated system. This tuning enhances the chemical stability of these oligomers by reducing the energy gap, making them more conductive systems.

In order to check in that effect on the photovoltaic properties, we listed in Table 5 the theoretical values of open-circuit voltage  $V_{oc}$  and the difference between the LUMO energy levels of the studied oligomers and those of the PC<sub>60</sub>BM. They have been calculated respectively from the following expressions (1 and 2) [14].

$$V_{oc} = |E_{HOMO}^{Donor}| - |E_{LUMO}^{Acceptor}| - 0.3 \quad (1)$$

$$\alpha = |E_{LUMO}^{Acceptor}| - |E_{LUMO}^{Donor}| \quad (2)$$

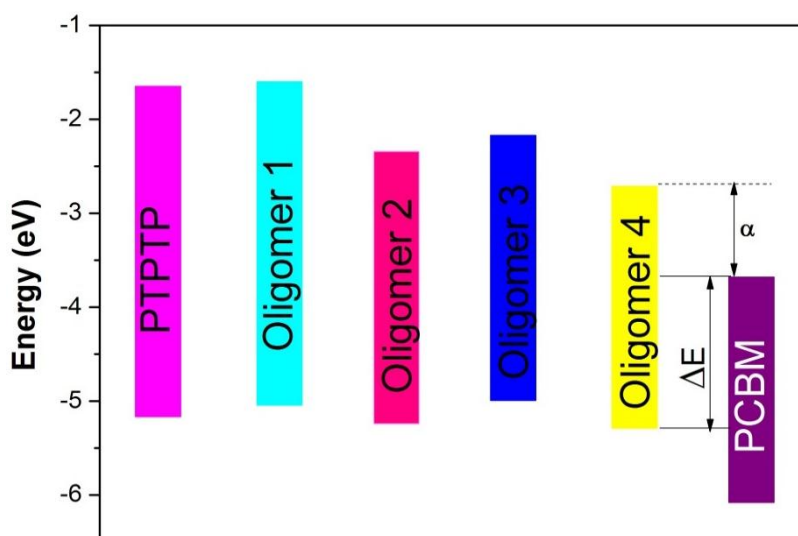
**Table 5:** Energy values of HOMO (eV), LUMO (eV), Eg (eV), open circuit Voltage  $V_{oc}$  (eV) and  $\alpha$  (eV) of oligomers

Oligomer	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	$E_{gap}$ (eV)	$V_{oc}$ (eV)	$\alpha$ (eV)
PTPTP	-5.16	-1.69	3.47	1.16	2.01
Oligomer 1(COCH <sub>3</sub> )	-5.06	-1.60	3.46	1.06	2.1
Oligomer 2 (CN)	-5.22	-2.33	2.89	1.22	1,37
Oligomer 3(COOH)	-4.99	-2.17	2.82	0.99	1,53
Oligomer 4(NO <sub>2</sub> )	-5.30	-2.73	2.57	1.30	0,97
PC <sub>60</sub> BM	-6.10	-3.70			

The fig. 7 shows the location of the HOMO and LUMO levels of each organic material; we can see that the PTPTP and oligomer 1 have the largest band gaps and values of  $\alpha$ .

The oligomers 2 and 3 have almost the nearly similar  $E_g$  with the difference in 0,07 eV, But the HOMO, LUMO levels site better for oligomer 2 than oligomer 3 ,allowing to rise the  $V_{oc}$  and decrease the  $\alpha$  value for oligomer 2.

On top of that the oligomer 4 has the most perfect photovoltaic properties, in as much as the lowest values of band gap 2,57 eV and of  $\alpha = 0.97\text{eV}$  , together with the highest  $V_{oc}$  (1.30eV). These results lead us to suggest that the photoexcited electron transfer from the LUMO level of the molecules to PC<sub>60</sub>BM may be sufficiently efficient to be useful in photovoltaic devices [15].



**Figure 7:** Band structure diagram illustrating the HOMO and LUMO energies of all oligomers with relative to the band structure of PC<sub>60</sub>BM.

#### 4. Conclusion:

In this article, the quantum chemical investigations on the geometries and electronic properties of several compounds based on thiophene and phenylene are performed to display the effect of acceptor and donor groups and the ring structure on the structural and optoelectronic properties of these materials. Five oligomers have been studied: unsubstituted, substituted with acceptor and donor groups. The substitution of electron-donating methoxy groups on the extreme phenylene rings and of electron-withdrawing groups (COCH<sub>3</sub>, CN, COOH, NO<sub>2</sub>) on the middle phenylene ring stabilize the HOMO and LUMO levels with a decrease in the energy gap. Therefore the nature of the acceptor/donor groups studied makes it possible to tailor the HOMO/LUMO positions with those of PC<sub>60</sub>BM so as to optimize them for photovoltaic applications. From this study, it can be concluded that the oligomer 4 is promising for these photovoltaic applications.

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