



Original Research article

# Electro-Optical and Photovoltaic Properties of Oligothiophene and Derivatives; Experimental and Theoretical Investigations



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## KEYWORDS

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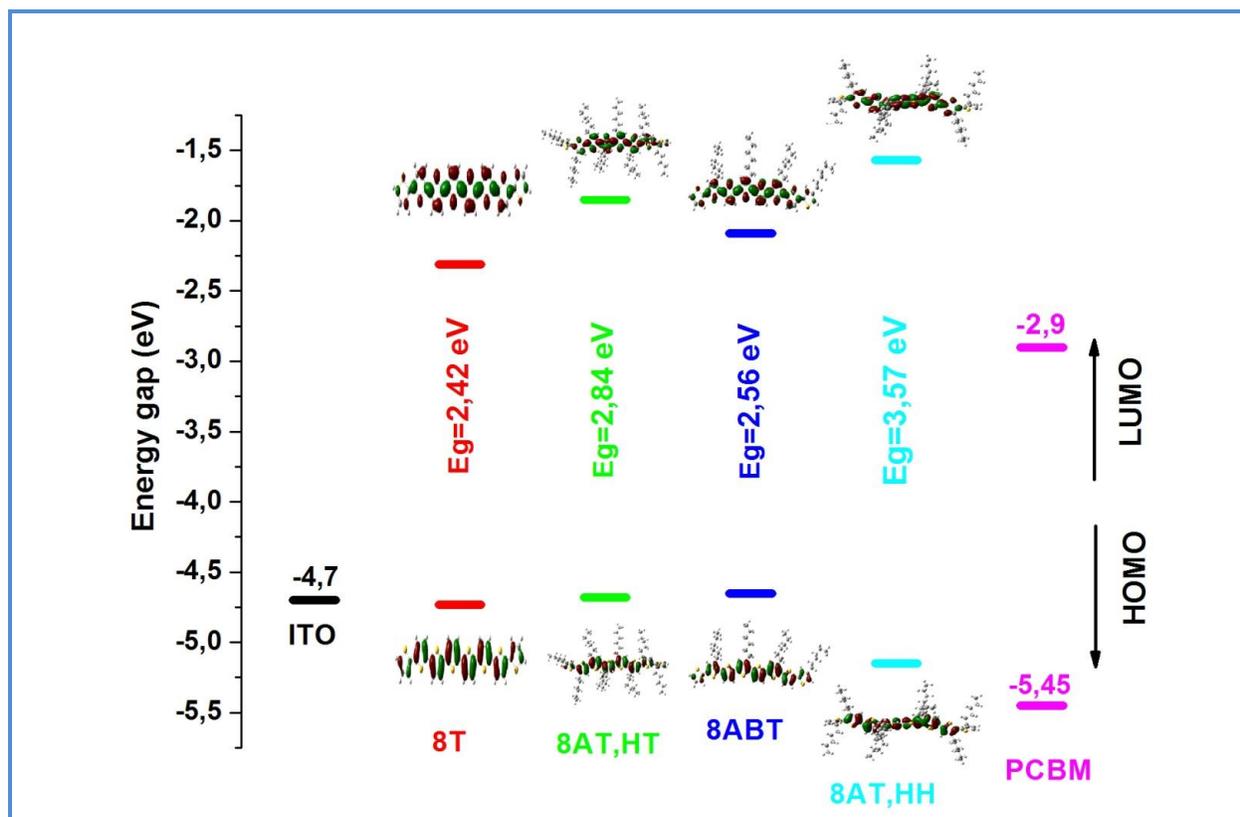
Organic solar cells

## ABSTRACT

In this work, conjugated polymers based on thiophene: polythiophene, poly (3-alkylthiophene) and poly (alkylbithiophene) were characterized using the nuclear magnetic resonance (NMR) and UV spectroscopy to determine their spectroscopic properties. Then, their structural, electronic and vibrational properties were investigated using the density functional theory (DFT) calculations by the oligomeric approach. The optoelectronic properties were assessed, as well. The obtained results were discussed basing on the influence of substitution on the properties of the oligomers. The possibility of thiophene based oligomers photovoltaic application was also studied. We have shown that the octithiophene (8T) its derivatives have a very good conversion rate and it serves as a candidate for the photovoltaic application.

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## Graphical Abstract



## Introduction

Conjugated polymers have been widely studied by several researchers over many years [1, 2]. These new materials discovered in 1977 by A.J. Heeger [3]. The main idea of the work was to investigate the dramatic increase of the conductivity of polyacetylene doped with iodine. The obtained results have opened up perspectives for many industrial applications such as for the conception of new organic photovoltaic cells and blue-emitting material for OLED and organic field-effect transistors [4, 5]. Among the various conjugated polymers, polythiophene has gained an increasing interest due to its stability. Despite of the various applications of polythiophene, its low solubility posed a significant technical hurdle to respond to different requirements and greatly limited its industrial development. The substitution of hydrogen at position 3 with an alkyl group could provide a straightforward avenue for improving the solubility of polythiophene. Then, a new class of conjugated polymers named poly (3-alkylthiophene), soluble in many organic solvents, is obtained [6-8]. These advanced materials that display a wealth of appealing properties were studied by several physicochemical techniques. Specifically, the use of solution characterization

techniques allowed a good identification of the sequences in the polymer chain [9]. Furthermore, since alkyl chains were found to play an important role in the molecular properties and spectral characteristics of poly (alkylthiophene) it is indispensable to obtain a thorough knowledge of the structure and backbone of the polymer chains.

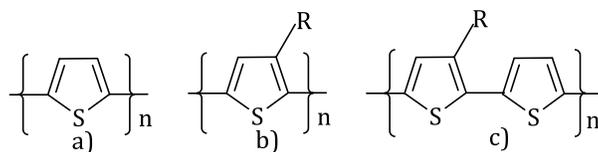
The present work discusses a theoretical evaluation of the geometric, optoelectronic, absorption, and photovoltaic properties of polythiophene (8T), poly (3-alkylthiophene) (8AT) and poly (alkylbithiophene) (8ABT) (Figure 1). The thiophene based oligomers were designed by introducing various alkyl groups. The impact of alkyl grafting on the thiophene ring and the regularity of sequences on physicochemical properties were investigated. We have focused our attention on improving these properties to make the studied oligomers excellent candidates for applications in organic devices such as the organic light emitting diode and organic solar cells.

The reported thiophene-based oligomers showed excellent photovoltaic properties including, the weak energy gap, high visible absorption, and low HOMO energy level which can boost the open circuit voltage  $V_{OC}$  value. Thanks to these interesting properties, these oligomers have been the subject of many diverse industrial applications especially in the field of organic electronics.

## Experimental

### Materials (bibliographic synthesis)

In this work, three thiophene-based polymers were studied (Figure 1).

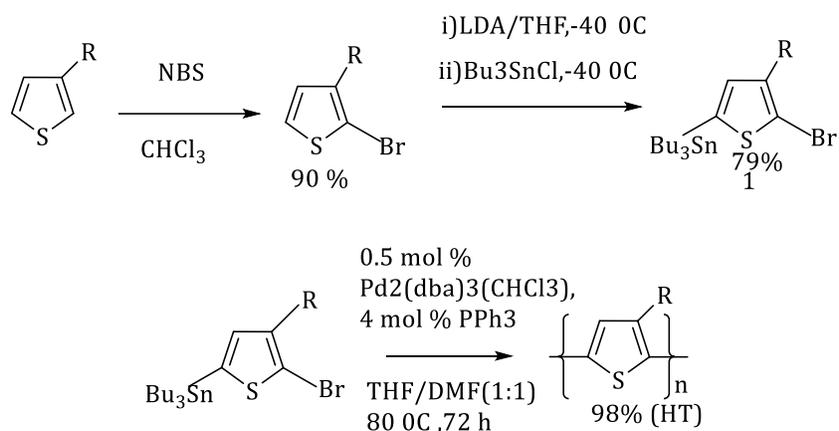


**Figure 1.** Chemical structures of the studied polymers: a) Polythiophene (PT), b) Poly (3-alkylthiophene) (PAT), and c) Poly (alkylbithiophene) (PABT)

The first work on polythiophene (PT) has been published by Yamamoto *et al.*, [10]. They have synthesized the PT by using polycondensation of 2,5-dibromothiophene using coupling magnesium in the tetrahydro furan (THF). Polythiophene has attracted significant attention for technological applications because of its interesting electron-transport and nonlinear optical properties. However, it remains completely insoluble and infusible due to the rigidity of its chain [11, 12]. Many attempts were taken to increase its solubility by amending several parameters in the chemical reaction. A viable and promising approach to the maximization of

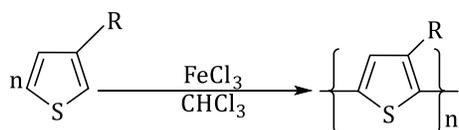
the efficiency of polythiophene is by grafting an alkyl group on position 3 of thiophene ring [13]. The poly (3-alkylthiophene) has been prepared by numerous teams according to different experimental protocols, either by chemical or electrochemical polymerization, or by organometallic synthesis [14]. It is worthy to note that two types of sequences are generated after substitution by an alkyl: the regular one named head-to-tail (HT) and the irregular one named head-to-head (HH). Let's remember that:

- Poly (3-alkylthiophene) (with 98% of HT) has been prepared by applying the palladium-catalyzed coupling procedure [15], according to Scheme 1:



**Scheme 1.** Organometallic synthesis of poly (3-alkylthiophene) [15]

Direct oxidation of the monomer with ferric chloride ( $\text{FeCl}_3$ ) represented by Scheme 2, leads to the formation of poly (3-alkylthiophene) having both the regular HT and irregular HH fragments with an important proportion of HT sequences [16].

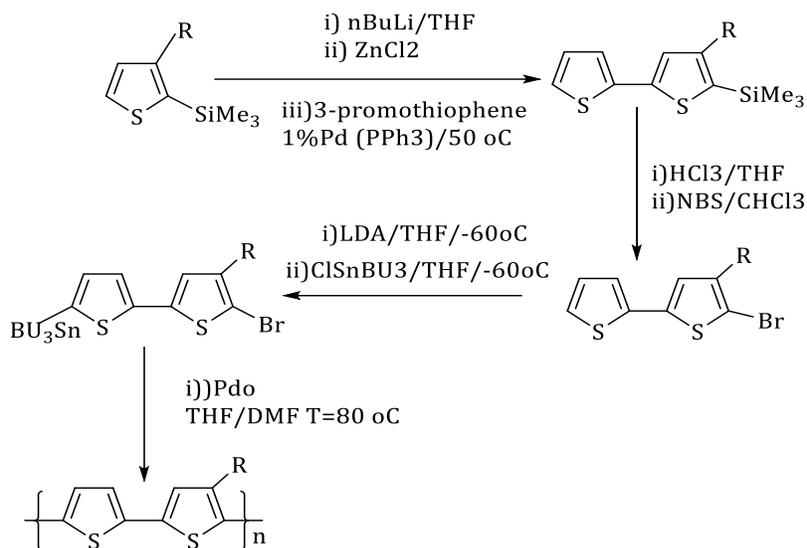


**Scheme 2.** Oxidation synthesis of poly (3-alkylthiophene) [16]

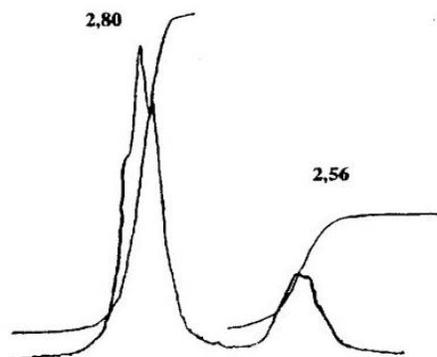
For poly (alkylbithiophene), it was prepared according to the method adopted by J.P. Lère-Porte *et al.*, [17], as represented in Scheme 3.

The rate of regularity which represents the percentage of pathways HT present in the polymer chain can be identified by  $^1\text{H}$  NMR analysis. Indeed, in the aromatic protons region (6.7-7.1 ppm) the protons of the regular sequences HT appear in 6.98 ppm while the corresponding

protons to the irregular chains (HH or TT) appear between 7 ppm and 7.05 ppm. On the other hand, to deduce the proportion of (HT) and (HH) sequences detected at 2.8 and 2.58 ppm respectively, in  $^1\text{H}$  NMR spectrum, an integration of the signals associated with the first  $\text{CH}_2$  of alkyl is performed (Figure 3).



**Scheme 3.** Synthesis of poly(alkylbithiophene) [17]



**Figure 2.** Signals corresponding to the protons of  $\alpha\text{CH}_2$  of the alkyl chain

#### According to its $^1\text{H}$ NMR spectrum

- ✓ Poly (3-alkylthiophene) obtained from the polycondensation of palladium, has 5% tail-to-tail (HH)
- ✓ Poly (3-alkylthiophene) obtained by electrochemical polymerization starting from 3-alkylthiophene leads to a polymer with 25% (HH) and an absorption maximum  $\lambda_{\text{max}} = 438\text{ nm}$ ,

- ✓ Poly (3-alkylthiophene) obtained by electrochemical polymerization starting from 4,4'-dialkyl-2,2' bithiophene leads to a polymer 100% (HH) and an absorption maximum  $\lambda_{\max} = 390$  nm
- ✓ A selective method developed by Lere-Porte *et al.*, [18] allowed to obtain a polymer with polymer with only 2% chain defects (HH) and an absorption maximum  $\lambda_{\max} = 515$  nm. The same percentage was obtained by Reicke *et al.*, [14-19].

These results revealed that the position of the maximum absorption ( $\lambda_{\max}$ ) strongly depends on the proportion of sequences [20-25]. When the polymer contains head-to-head chaining defects (HH), the value of  $\lambda_{\max}$  is lower and the material loses in conjugation (Table 1). This is explained by the superabundance of the alkyl chains and therefore, the (HH) chain defects lead to steric constraints. The polymer adopts in this case conformations, leading to a rupture of the conjugation and a degradation of the electro-active properties of the polymer.

**Table 1.** Various types of selective synthesis of poly (3-hexylthiophene) and influence of the percentage of HH

Monomer	Type of polymerization	%HH	$\lambda_{\max}$ (CHCl <sub>3</sub> )
2-bromo-5-tributylstannyl-3-hexylthiophene	Palladium-catalyzed coupling	2%	515 nm
2-bromo-5-iodo-3-hexylthiophene	Zinc catalyzed coupling	2%	460 nm
3-hexylthiophene	Chemical or electrochemical oxidation	30%	438 nm
4,4'-dihexyl-2,2'-bithiophene	Electrochemical oxidation	100%	390 nm
3,3'-dihexyl-2,2'-bithiophene	Chemical oxidation	100%	384 nm

### Methods of quantum chemistry

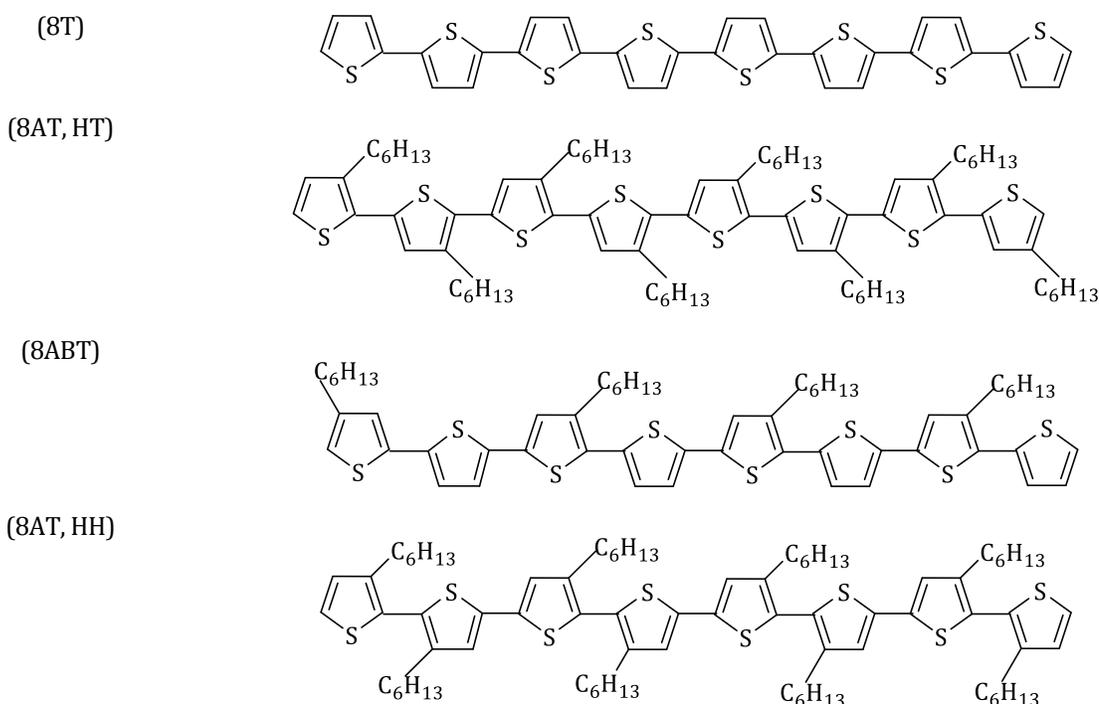
All the molecular calculations were performed in gas phase using the Gaussian 09 program [26]. The optimizations were performed using the DFT/B3LYP with 6-31G (d, p) basis set for all atoms [27-29]. The calculation of vibration frequencies for each molecule revealed that there are no imaginary frequencies. This confirms that the optimized geometry is located at a minimum point of the potential surface. The long range coulomb-attenuating method (CAM-B3LYP) [30] has been applied to predict the excitation energies and the absorption spectra of conjugated molecules. In this work the vertical excitation energy and electronic absorption spectra were simulated using the TD-CAM-B3LYP method [31]. The energy of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels were examined and visualized using the Gauss view software [32].

## Results and discussion

The computational study was based on an oligomeric approach already applied by many authors, especially by Bouzzine *et al.*, [33]. We consider as models 08 thiophene-based oligomers: (8T), (8AT, HT), (8ABT) and (8AT, HH) (Figure 6), and carry out a quantum study on them. We examined the geometric, electronic, optical and photovoltaic properties of these 4 models of the thiophene-based oligomers. To study the influence of alkyl groups' substitution on the latter properties, (8T) was taken as a reference oligomer. Our results on (8T) properties were in accordance with the results obtained by H. Nikoofard *et al.*, [34]. The gap energy was found to be 2.27 eV and the values of the simulated absorption spectra was  $\lambda_{\max}=559$  nm.

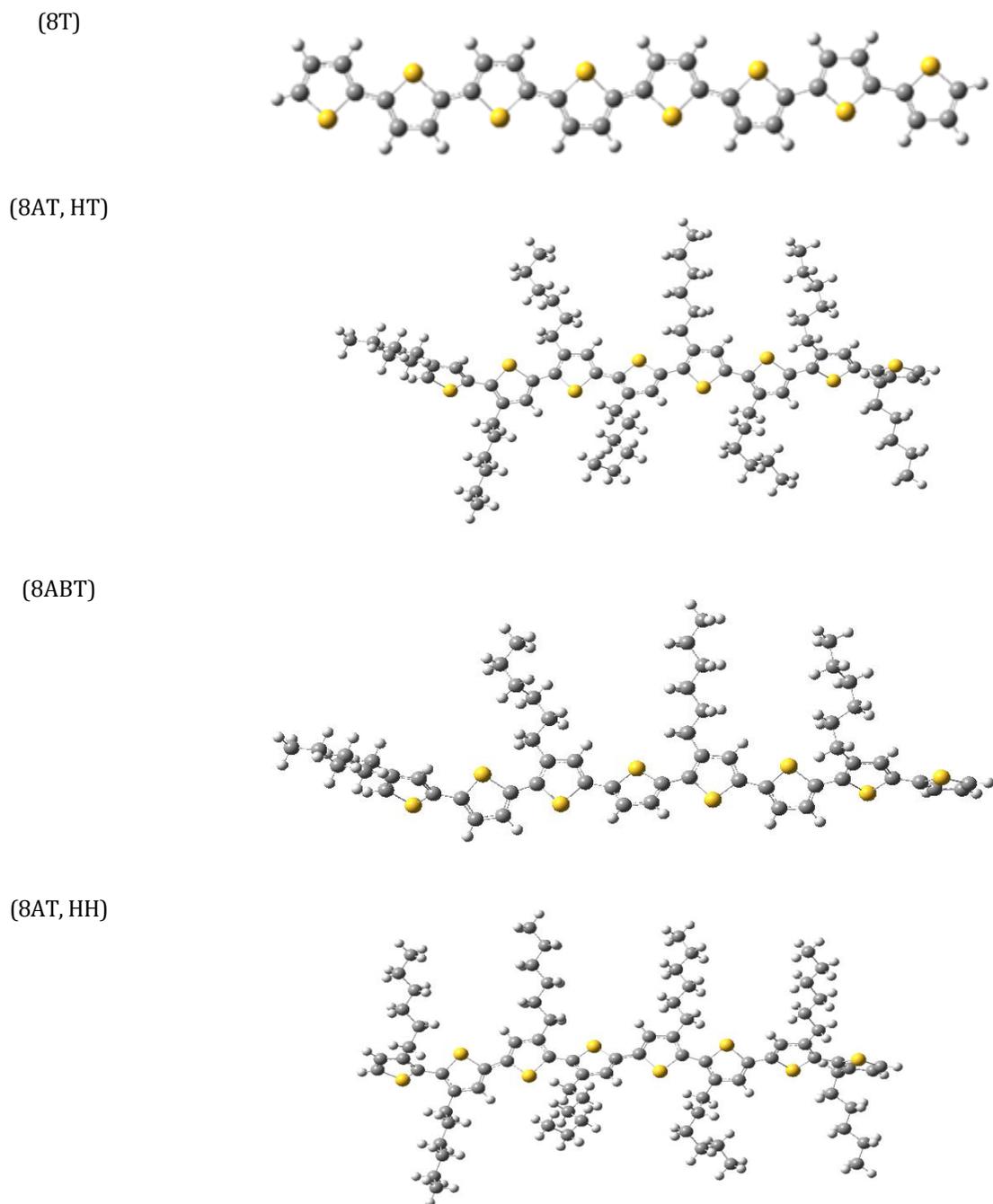
### Geometric properties

To assess the effect of the alkyl groups on the geometric properties of the studied thiophene-based oligomers, we have started by optimizing the structures using the B3LYP/6-31G method (d, p).



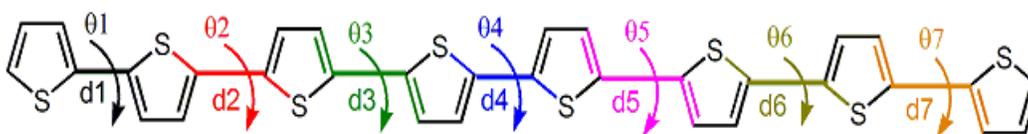
**Figure 6.** Chemical structures of thiophene-based oligomers (8T), (8AT, HT), (8ABT), and (8AT, HH)

To study the impact of grafting alkyl groups on the geometric and the electronic properties, the obtained structures of the four studied oligomers (8T), (8AT, HT), (8ABT) and (8AT, HH) obtained by B3LYP/6-31G (d, p) have been compared (Figure 7).



**Figure 7.** Optimized structures obtained by B3LYP/6-31G (d, p) of thiophene-based oligomers (8T), (8AT, HT), (8ABT) and (8AT, HH)

The selected dihedral angle  $\theta_i$  ( $i=1-7$ ) and the inter-ring distance parameters  $d_i$  ( $i=1-7$ ) are depicted in Figure 8, Tables 3 and 4.



**Figure 8.** Scheme of the bond  $d_i$  ( $i=1-7$ ) lengths and dihedral angles  $\theta_i$  ( $i=1-7$ )

**Table 3.** Inter-ring distances  $d_i$  (Å)

Inter-ring distances (Å°)	d1	d2	d3	d4	d5	d6	d7
(8T)	1.446	1.441	1.441	1.441	1.441	1.441	1.446
(8AT,HT)	1.457	1.449	1.449	1.449	1.451	1.452	1.454
(8ABT)	1.447	1.449	1.442	1.445	1.442	1.448	1.447
(8AT,HH)	1.466	1.449	1.464	1.449	1.464	1.449	1.466

**Table 4.** Dihedral angles  $\theta_i$ (°)

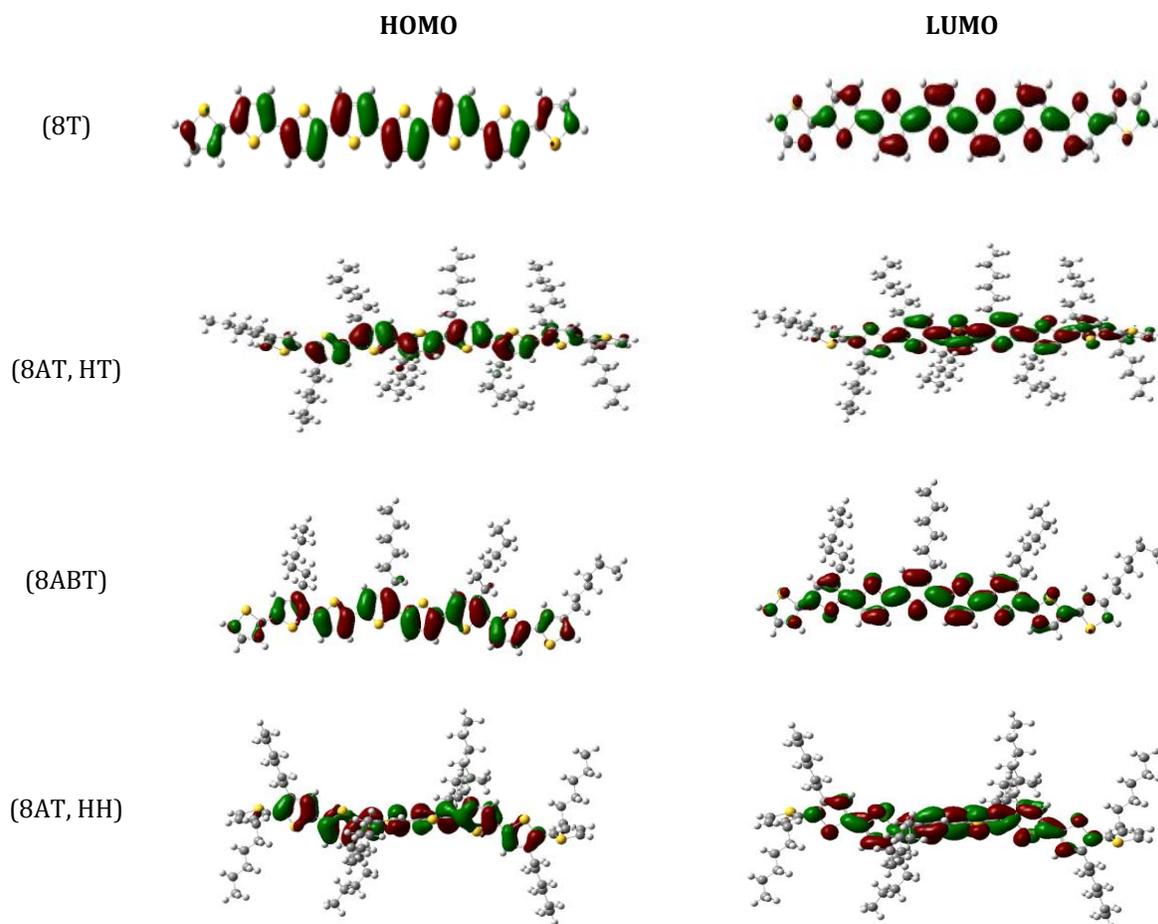
Dihedral angles ( $\theta^\circ$ )	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$	$\theta_5$	$\theta_6$	$\theta_7$
(8T)	179.97	-179.98	179.98	-179.99	179.99	-179.99	179.97
(8AT, HT)	139.51	156.73	154.90	-151.83	-149.59	-149.95	-150.61
(8ABT)	161.86	-151.08	166.75	-162.88	177.09	153.75	-164.02
(8AT, HH)	-106.01	-168.42	168.59	-167.31	108.01	161.44	102.29

Theoretical calculations depicted that the obtained torsion angles adopt a value of approximately 180° for (8T) (a quasi-planar conformation). In the rest of oligomers structures, the dihedral angles evolved toward an anti-gauche conformation with  $\theta$  varying in the ranges 139.51°-156.73°, 151.08°-177.09°, and 102.29°-168.59° for (8AT, HT), (8ABT) and (8AT, HH), respectively. By comparing the geometrical parameters of the studied thiophene-based oligomers especially the torsion angles values, it was found that the insertion of the alkyl groups significantly may cause a distortion between the thiophene rings, and subsequently the structures, hence the variation of the electronic properties of parent polymers. These results can be explained by the repulsion of alkyl groups which promote the fragility of the compounds. Furthermore, it is worthy to note the existence of a strong attraction between alkyl groups, proved by an increase of HH irregular sequences in substituted oligomers (8AT, HT), (8ABT) and (8AT, HH) respect to those of (8T).

### Electronic properties and frontier molecular orbital

It is important to examine HOMO and LUMO orbitals for these molecules, because the relative scheduling of the occupied and virtual orbit provides a reasonable qualitative indication of the excitation properties [35]. For that, the HOMO and LUMO energy levels of our studied compounds (8T), (8AT, HT), (8ABT) and (8AT, HH) have been examined. As indicated in Figure 9, the HOMO

had an anti-bonding character between the consecutive subunits, while the LUMO showed a binding character between the subunits.



**Figure 9.** Calculated FMOs for all the molecules examined

The energy values  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$ , and  $E_{\text{gap}}$  were theoretically evaluated from the optimized geometries obtained by B3LYP/6-31G (d, p). The obtained data are summarized in Table 5, comparing these theoretical energies values to those measured practically, a slight difference was clearly observed. This can be due to the fact that the calculations are supposed to be made in gaseous states.

The results revealed that the polythiophene has the lowest HOMO-LUMO energy gap of 2.42 eV. For the substituted oligomers, the energy gap values were increasing in the following order  $E(8\text{ABT}) < E(8\text{AT, HT}) < E(8\text{AT, HH})$ . The increase in the energy gap might be due to the insertion of the alkyl chains which causes the distortion of the aromatic cycles with a non flatness of the structure and consequently a bad conjugation. Therefore, as expected, the lowering of the HT chains induces a

rise of the HOMO-LUMO energy gap which confirms that the regularity of the sequences has an effect on the electronic properties. Indeed, excellent electronic properties were detected for polythiophene with regular sequences (HT): (8AT) with 100% HT, possesses an energy gap of 2.84 eV while a value of 3.57 eV was recorded for the same polymer with 0% HT. This reveals the existence of repulsive forces between the groups which appear clearly in the molecule (8AT, HH) having the highest gap energy. Consequently, the conformational structure is modified, producing a decrease in the mobility of charges, followed by a recombination of charges in the active layer and hence a lower free carrier density.

### Photovoltaic properties

The bulk heterojunction BHJ cells consisting of polythiophene as donor and PCBM (or these derivatives) as acceptor have many advantages such as low manufacturing cost and easy processing. The organic solar cells based on these molecules have been attracting much attention by many researches [36]. Efficiency of the  $\pi$ -conjugated compounds as photovoltaic devices can be estimated by calculating the power conversion efficiency (PCE) which measures the amount of power produced by a solar cell relative to the power available in the incident solar radiation ( $P_{inc}$ ). The photovoltaic cell efficiency (power conversion efficiency ( $\eta$ )), can be calculated using Equation 1 [37].

$$\eta = FF \frac{V_{oc} J_{sc}}{P_{inc}} \tag{1}$$

Where  $P_{inc}$  is the incident power density,  $V_{oc}$  is the open-circuit voltage,  $J_{sc}$  is the short-circuit current, and  $FF$  is the fill factor. The theoretical values of the open-circuit voltage  $V_{oc}$  were calculated using Equation 2 [38].

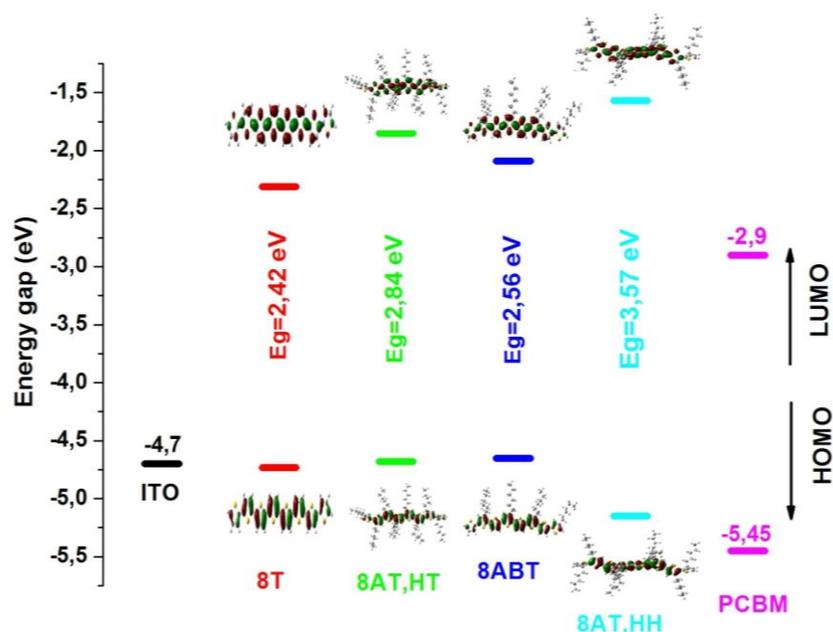
$$V_{oc} = \frac{1}{e} (|E_{HOMO}(Donor)| - |E_{LUMO}(Acceptor)| - 0.3) \tag{2}$$

**Table 5.** The values of the energy,  $E_{LUMO}$  (eV),  $E_{HOMO}$  (eV),  $E_{gap}$  (eV) and the open circuit voltage  $V_{oc}$  (V)

Compounds	$E_{HOMO}$	$E_{LUMO}$	$E_{gap}$	$E_{gap}^{* exp}$	$V_{oc}$ (V)	$\alpha$ (eV)
(8T)	-4.73	-2.31	2.42	2.3	1.53	0.59
(8AT, HT)	-4.68	-1.85	2.84	-	1.48	1.05
(8ABT)	-4.65	-2.09	2.56	-	1.45	0.81
(8AT, HH)	-5.15	-1.57	3.57	-	1.95	1.32
2.4.6-OMe-PCBM**	-5.45	-2.90				

\* [33]

\*\*[39]



**Figure 10.** Energy gap and frontier molecular orbital energy levels of PCBM and thiophene-based oligomers (8T), (8AT, HT), (8ABT) and (8AT, HH)

The  $V_{oc}$  values calculated by Equation 2 were ranging from 1.53 V for (8T), to 1.95 V for (8AT, HH) when considering 2.4.6-OMe-PCBM as an acceptor (Table 5).

To achieve an effective injection of the electron into the conduction band of 2.4.6-OMe-PCBM, the difference between the LUMO energy of the donor (oligomer) and the LUMO energy of the acceptor must be positive.

$$\alpha_i = E_{HOMO}(\text{Donor}) - E_{LUMO}(\text{Acceptor}) \quad (3)$$

As seen in Table 5, all  $\alpha_i$  values of the studied thiophene-based oligomers (8T), (8AT, HT), (8ABT) and (8AT, HH), are positives. This indicates that such molecules can be used as organic solar cells since their process of electron injection to the conduction band of 2.4.6-OMe-PCBM and the subsequent regeneration are feasible.

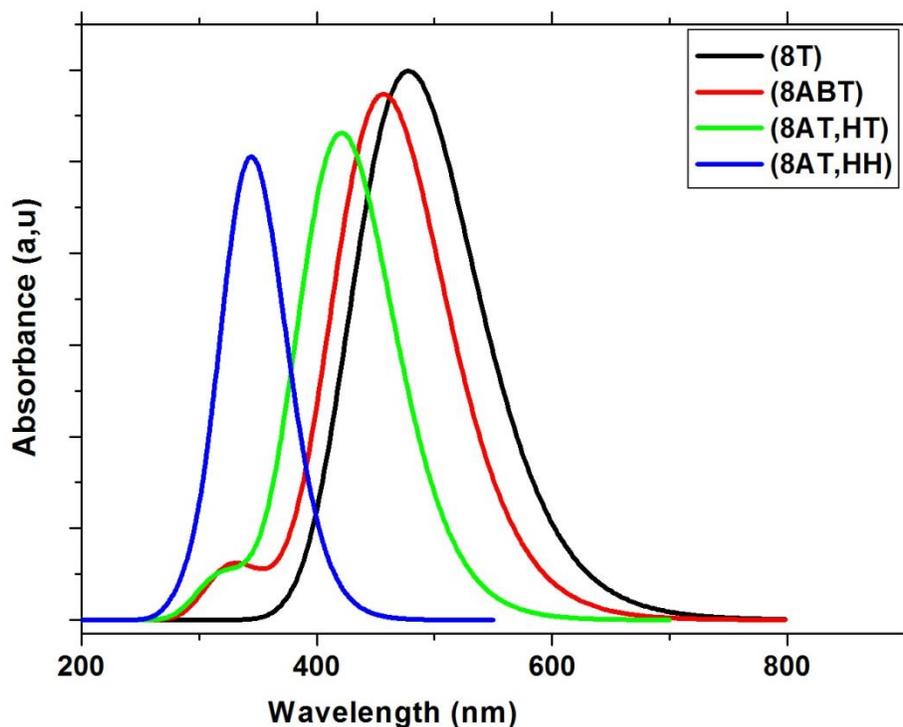
On the other hand, the optical properties, electronic transition, excitation energy and UV/Vis absorption spectra of the all studied oligomers were performed using CAM/(B3LYP)/6-31G (d) calculations. The results of the excited singlet states, transitions energies, oscillator strength (O.S) and absorption spectra of all studied molecules are shown in Table 6. The spectra shown in (Figure 11) exhibited similar profiles for all compounds. They display a main intense band at higher energies in the visible region ranging from 345.21 nm for (8AT.HH) to 478.05 nm for (8T). These strong absorption peaks were assigned to the intramolecular charge transfer (ICT) transitions, and

arise from S0 to S1, which corresponds to the dominant promotion of an electron transition from HOMO to LUMO.

From the results recorded in Tables 3 and 4, contrary to polythiophene, the compounds (8ABT), (8AT, HT) and (8AT, HH) present non planar conformations; this confirms the existence of the steric effects exerted by the alkyl groups. In other works, greater are the steric interactions, weaker the conjugation is. These features are corroborated by the observed increase of the maximum wavelength absorption value  $\lambda_{\max}$  for the oligomers studied by decreasing the percentage of linear alkyl chains in this order:  $\lambda_{\max}(\text{8AT, HT}) > \lambda_{\max}(\text{8AT, HH}) > \lambda_{\max}(\text{8ABT}) > \lambda_{\max}(\text{8T})$ .

**Table 6.** Absorption maximum  $\lambda_{\max}$ , activation energy,  $E_{\text{activation}}$  oscillator strength and M/O character of the thiophene-based oligomers studied, obtained by CAM-B3LYB calculations

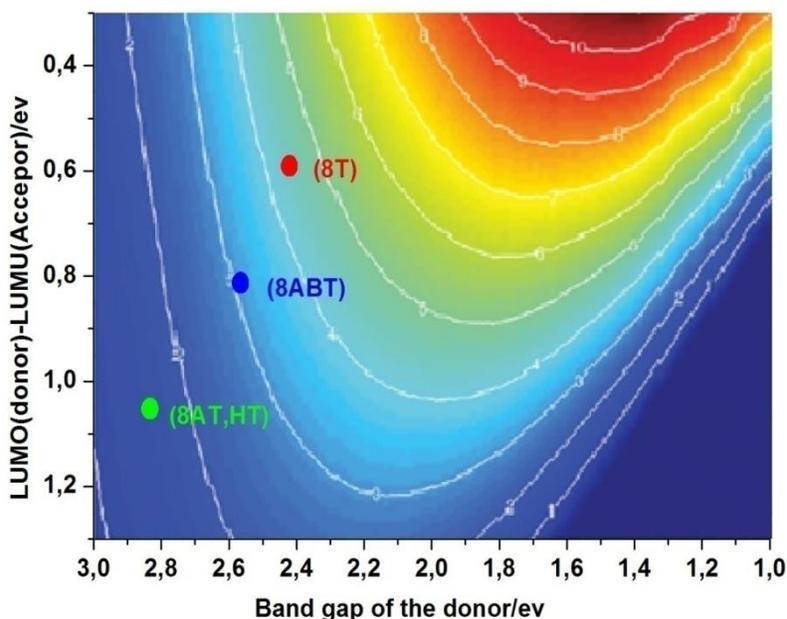
Compounds	$\lambda_{\max}$ (nm) CAM-B3LYB	$E_{\text{activation}}$ (eV)	O.S	MO/character
(8T)	478.05	2.59	2.96	HOMO→LUMO (81%)
(8AT, HT)	421.39	2.94	2.62	HOMO→LUMO (80%)
(8ABT)	457.05	2.71	2.83	HOMO→LUMO (82%)
(8AT, HH)	345.21	3.59	2.45	HOMO→LUMO (69%)



**Figure 11.** Theoretical UV-visible optical absorption spectra of thiophene-based oligomers (8T), (8AT, HT), (8ABT) and (8AT, HH), plotted from data obtained using the CAM/B3LYP method

Generally, semiconductor organic materials have a low dielectric constant ( $\epsilon \approx 3$ ) and a very high absorption coefficient of ( $>10^5 \text{ cm}^{-1}$ ). Biological semiconductor could be classified according to its molecular weight and its gain or loss capacity of electrons. Biological semiconductor can be distinguished as small molecule or polymer and as electron donor or electron acceptor. In case of the last classification, when a photon is absorbed by an electron donor, the electron is excited to an excited state of energy. It binds with the holes to form exciton with a binding energy of about 0.3-0.4 eV. The latter is then scattered at the interfaces between the electron donor and acceptor under the integrated electric field and will be dissociated into free charge carriers. That will be collected by their corresponding electrodes. Based on Scharber model [40], the maximum power conversion efficiency of the photovoltaic solar cell for the compound (8T)/2,4,6-OMe-PCBM can be attained 5% (see Figure 12).

The compound (8T) showed the best conjugation properties and it can be a candidate for the photovoltaic application. However its insufficient solubility limits the application. Such an issue is solved by substituting (8T) by alkyl groups. So, (8AT, HT) was found to exhibit interesting photovoltaic properties. In general and according to the results obtained (weak gap, high visible absorption,  $V_{oc}$  value and solubility), the thiophene oligomers and derivatives are excellent candidates for applications (LEDs, transistors, photovoltaic ones).



**Figure 12.** Contour plots showing the energy-conversion efficiency of the investigated polymers

## Conclusion

We have carried out quantum chemical calculations at DFT level of a series of thiophene-based oligomers.

6-31G (d, p) basis set was used to perform geometry optimizations and vibrational analysis of the oligomers. DFT calculation corroborates with the data obtained by NMR and UV. DFT calculation revealed that the presence of irregular sequences head-to-head (HH) affects importantly the conjugation of the polymer due to the steric interactions exerted by the alkyl chains. Compared to the oligomer with head-to-head sequences (8AT, HH), the oligomer (8AT, HT) exhibited greater value of the maximum wavelength absorption  $\lambda_{\max}$ . Conversely, lowering of the HT chains induces a rise in the HOMO-LUMO energy gap.

The results demonstrated that, the electronic and optical properties of the oligomers can be significantly improved by changing the number of alkyl groups and the regularity of sequences.

To assay the efficacious employ of the studied thiophene-based oligomers in the solar cell applications, the Scharber model has been followed. The oligomer (8T) revealed a very good conversion rate and served as a candidate for the photovoltaic application. Its substitution by alkyl groups to overcome the issue of its low solubility gives rise to the (8AT, HT) oligomer with interesting photovoltaic properties. It was also found that the grafting by alkyl groups is an effective way to design new materials with properties of photovoltaic cells.

Finally, it is recommended that the systematic use of DFT approach can predict the optoelectronic properties on various oligomers, which helps to understand the structure-properties relationship of these systems, and further to design novel materials suitable for high performance for organic solar cell devices.

## Conflict of Interest

We have no conflicts of interest to disclose.

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