African Journal of Pure and Applied Chemistry Vol. 6(14), pp. 164-172, December 2012
Available online at http://www.academicjournals.org/AJPAC
DOI: 10.5897/AJPAC12.021
ISSN 1996 - 0840 ©2012 Academic Journals

Full Length Research Paper

New compounds based on anthracene as a good candidate for organic dye-sensitized solar cells: Theoretical investigations

N. Belghiti[1], M. Bennani[1], M. Hamidi[2], S. M. Bouzzine[2] and M. Bouachrine[3]*

[1]Laboratoire de Recherche «Chimie-Biologie appliquées à l'environnement», Faculté des Sciences, Université Moulay Ismail Meknès, Marocco.
[2]URMM/UCTA, Faculté des Sciences et Techniques d'Errachidia, Université Moulay Ismaïl, Maroc
[3]ESTM, Université Moulay Ismail, Meknes, Marocco.

Accepted 7 June, 2012

The specific properties of organic-conjugated molecules and polymers are of great importance since they have become the most promising materials for the optoelectronic device technology such as solar cells. The use of low band gap materials is a viable method for better harvesting of the solar spectrum and increasing its efficiency. The control of the parameter of these materials is a research issue of ongoing interest. In this work, quantum chemical investigation was performed to explore the optical and electronic properties of a series of different compounds based on anthracene. Different electron side groups were introduced to investigate their effects on the electronic structure. The 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 the HOMO, LUMO, Gap energy and open circuit voltage (Voc) of the studied compounds have been calculated and reported. These properties suggest these materials as good candidate for organic dye-sensitized solar cells.

Key words: π-Conjugated molecules, anthracene, organic solar cells, density function theory (DFT), low band-gap, electronic properties.

INTRODUCTION

The π-conjugated molecules and polymers based on heterocylcic ring and characterized by an extended π-conjugation is of broad interest in many areas of research, for their applications in organic electronics (Nalwa, 1999; Lim et al., 2006). Particularly in the last decade, optoelectronic device technology (Nalwa, 1999; Lim et al., 2006), such as light-emitting diode (LEDS) (Dimitrakopolous and Malenfrant, 2002), thin film transistors (TFTs) (Kraft et al., 1998; Kim et al., 2006) and low-cost solar cells (Manoj and Narayan, 2003; Wienk et al., 2003) are among these applications. Obtained polymers are highly amorphous, while oligomers are not amorphous and can be synthesized as well defined compounds. Recently, many researchers have become interested in synthesizing short-chain organic OLED compounds based on conjugated oligomers (Müllen and Wegner, 1998; Cornil et al., 1998).

Considerable efforts have been directed towards the study of the electro-optic properties of these conjugated systems, with the aim to exploit their potential as materials for stable and easy processable devices (Sariciftci et al., 1992; Brabec et al., 2001; Roquet et al., 2006). These materials offer advantages over polymeric systems in terms of easy synthesis and purification, and generally exhibit high charge carrier mobility. Therefore, designing and synthesizing molecules with interesting properties play a crucial role in technology (Bundgaard and Krebs, 2007; Brocks and Tol, 1996). At the same time, it is important to understand the nature of the relationship between the molecular structure and the

---

*Corresponding author. E-mail: bouachrine@gmail.com.

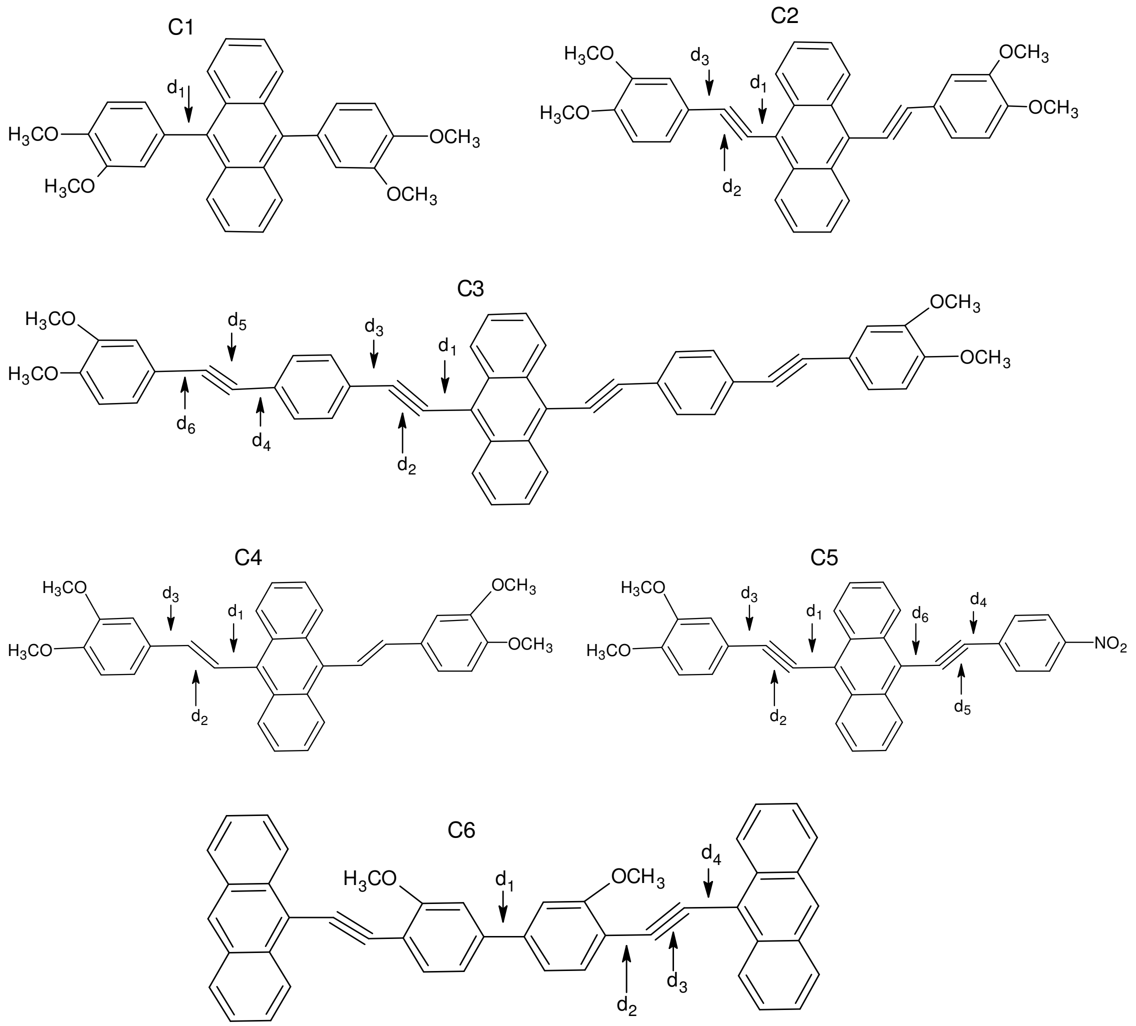

Figure 1. The sketch map of studying structures (C1, C2, C3, C4 C5 and C6).

electronic properties to provide guidelines for the development of new materials. Recent work in this area has been focused on the synthesis and design of new molecules combining donor and acceptor blocks, or conjugated systems with narrow band gaps (Cravino et al., 2002). Theoretical analysis of the electronic structure of conjugated systems can establish the relationships between molecular structure and electronic properties.

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 of those yet unknown. In this context, quantum-chemical methods have been increasingly applied to predict the band gap of conjugated systems (Bouzakraoui et al., 2006; Bouzakraoui et al., 2005; Zgou et al., 2008; Bouzzine et al., 2008; Mondal et al., 2010). We note that theoretical knowledge of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels of the components is crucial in studying organic solar cells. So, we can save time and money by choosing the adequate organic materials to optimize photovoltaic device's properties. 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 properties of the organic solar cells.

Recently, Marrocchi et al. (2010) described the synthesis of a series of anthracene-containing semiconductors (Figure 1). Anthracene derivatives may exhibit large charge carrier mobility and excellent stability. To the best of our knowledge, a systematic theoretical study of such compounds has not been reported.

This work shall further elucidate geometric and electronic properties with the aim to evidence the relationship between molecular structure and electronic properties, thus, driving towards the next syntheses compounds useful as active

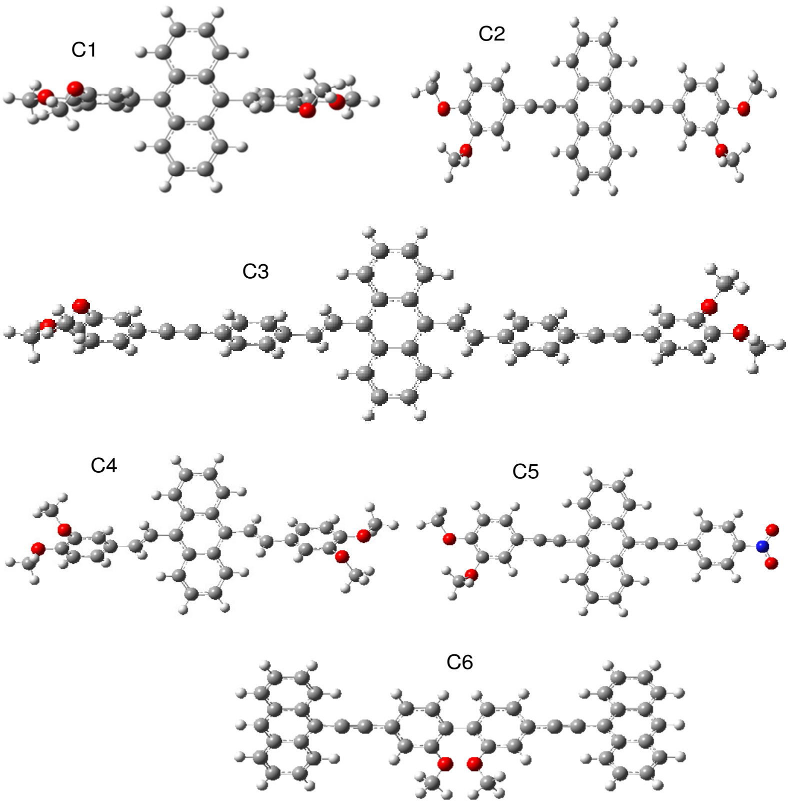

Figure 2. Optimized structure of C1, C2, C3, C4, C5 and C6 obtained by B3LYP/6-31(d) level.

materials in optoelectronic; the quantum chemical investigation has been performed to explore the optical and electronic properties of a series of different compounds based on anthracene. Different electron side groups were introduced to investigate their effects on the electronic structure. The theoretical knowledge of the HOMO and LUMO energy levels of the components is a basis in studying organic solar cells as the HOMO, LUMO and gap energy of the studied compounds have been calculated and reported. Their properties suggest they are good candidates for organic solar cells

THEORETICAL METHODOLOGY

Density function theory (DFT) method of three-parameter compound of Becke (1993) (B3LYP) was used in all the study of the neutral and polaronic compounds. The 6-31G(d) basis set was used for all calculations (Ditchfield et al., 1971; Hehre et al., 1972; Hariharan and Pople, 1974; Gordon, 1980). 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 (Frisch et al., 2003). The geometry structures of neutral and doped molecules were optimized under no constraint. We have also examined HOMO and LUMO levels; the energy gap is evaluated as calculated by the difference between the HOMO and LUMO energies. The ground state energies and oscillator strengths were investigated using the ZINDO/s, calculations on the fully optimized geometries. In fact, these calculation methods have been successfully applied to other conjugated polymers (Meille et al., 1994).

RESULTS AND DISCUSSION

Molecular design and geometry structures

The optimized structures of all studied compounds are shown in Figure 2. It reveals that the π-electron delocalization between the different aromatic units is clear. For the effect of increasing additional conjugated, π-bridge are studied. The addition of end alkoxy chains to backbone might increase the materiel solubility. In addition, molecules C2 and C5 are designed in order to examine the effect of asymmetry in comparison with the corresponding ones and also the effect of the electro accepting group (NO_2) and finally in order to examine the effect of the position of anthracene compounds, molecule C6 and C7 are designed. Finally, in order to study the effect of terminating anthracene moieties on the electronic properties, the doubled end-capped dianthryl compound C6 has also been considered. All the molecular geometries have been calculated with the Hybrid B3LYP function combined with 6-31G (d) basis

Table 1. Geometrical parameters of study compounds C1 to C6 obtained by B3LYP/6-31G(d) in their neutral (N) and doped (D) states.

Compound state	d_1(Å)	d_2(Å)	d_3(Å)	d_4(Å)	d_5(Å)	d_6(Å)
C1(N)	1.497					
C1(D)	1.474					
C2(N)	1.421	1.219	1.417			
C2(D)	1.404	1.227	1.394			
C3(N)	1.422	1.217	1.421	1.464	1.349	1.475
C3(D)	1.415	1.220	1.412	1.464	1.356	1.464
C4(N)	1.467	1.384	1.467			
C4(D)	1.447	1.367	1.445			
C5(N)	1.420	1.219	1.426	1.415	1.220	1.417
C5(D)	1.400	1.229	1.391	1.402	1.223	1.416
C6(N)	1.420	1.218	1.423	1.486		
C6(D)	1.405	1.220	1.411	1.472		

Table 2. Values of HOMO (eV), LUMO (eV) and Gap energy (eV) energies calculated for, C1 to C6 obtained by B3LYP/6-31G(d).

Compound	C1	C2	C3	C4	C5	C6	C7
HOMO-1	-6.75	-6.59	-6.66	-6.71	-6.85	-6.45	-6.61
HOMO	-4.95	-4.67	-4.80	-4.77	-5.11	-4.93	-4.86
GAP	3.47	2.57	2.78	2.95	2.35	2.90	2.20
LUMO	-1.48	-2.09	-2.02	-1.82	-2.75	-2.03	-2.65
LUMO+1	0.57	0.53	-0.002	0.35	-0.25	0.17	0.09

sets using GAUSSIAN 03 program. It was found in other works (Bouachrine et al., 2011) that the DFT-optimized geometries were in excellent agreement with the data obtained from X-ray analysis.

The results of the optimized structures for all studied compounds show that they have similar conformation (quasi planar conformation) (Figure 2). We found that the consecutive units have similar dihedral angles (180°) and inter-ring distances (d_1=1.424 Å, d_2=1.259 Å, d_3=1.387 Å, d_7=1.440 Å, d_8=1.3689 Å, d_9=1.482 Å) (Table 1). The incorporation of several groups does not change these parameters.

On the other hand, it is interesting to study how the p-doped π-conjugated molecule becomes the ultimate responsible of charge transport. As earlier said, to obtain oxidized optimized structure, we started from the optimized structure of the neutral form. We can conclude that during the doping process and for all studied compounds the simple bonds become shorter, while the double ones become longer. The inter-rings bonds are longer than normal double bonds. A quinoid-like distortion emerges as a result of the oxidation. These results are consistent with the ab-initio HF and DFT calculations performed by Casado et al. (1997) and Bouzzine et al. (2005) for substituting oligothiophenes. The optimized geometry of the cationic compound indicates the formation of the positive polaron defect localized in the middle of the molecule and extending over the adjacent repeat units. The charged species are characterized by a reversal of the single double C-C bond pattern; the geometry process thus induces the appearance of a strong quinoid character within the molecule.

Electronic parameters

Electronic structures are fundamental to the interpretation and understanding of the absorption spectra. The calculated frontier orbital energies (four occupied orbital and four unoccupied orbital) and energy gaps between HOMO and LUMO are shown in Table 2. As shown in Table 2, one can notice that all studied molecules (C2 to C6) exhibit destabilization of the LUMO and stabilization HOMO levels in comparison with those of compound C1. The HOMO and LUMO energies of C1 to C6 change significantly, (-4.96 and -1.48 eV, -4.67 and -2.09 eV, -4.80 and -2.02eV, -4.77 and -1.82eV, -5.11 and -2.76eV, and -4.93 and -2.03eV, respectively). It can also be found that, the HOMO and LUMO energies of the studied compound are slightly different. This implies that different structures play key roles on electronic properties and enhancing the electron-accepting ability and the effect of

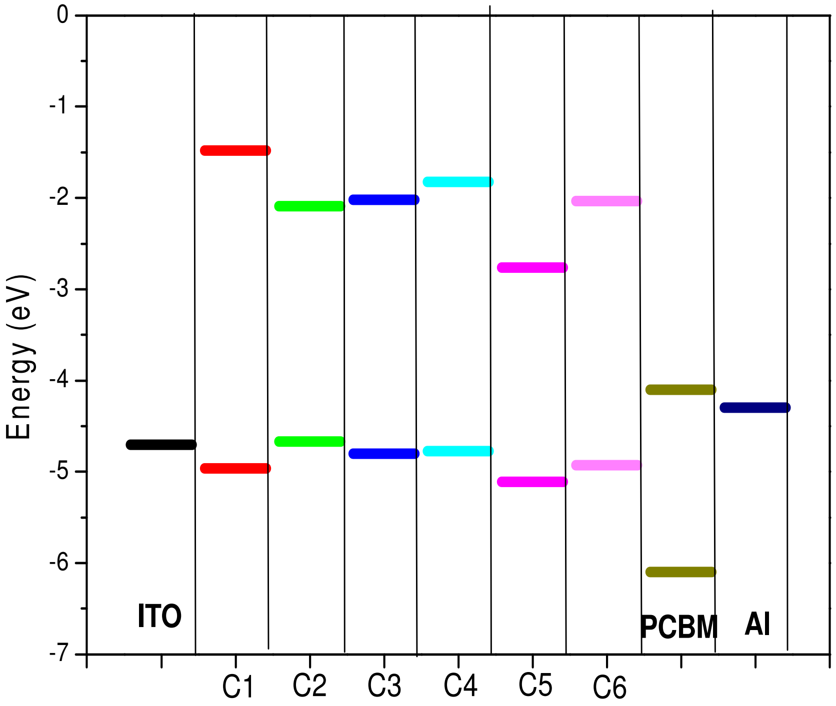

Figure 3. Data of the absolute energy of the frontier orbitals HOMO and LUMO for the studied molecules and ITO, PCBM and the aluminum (Al).

the symmetry of ethylene-thiophene branch on the HOMO and LUMO energies cannot be neglected. In addition, the energies of E_{gap} C1 to C6 differ slightly from 2.35 to 3.47eV depending on the different structures. They are studied in the following order C1 > C4 > C6 > C3 > C2 > C5.

It should be emphasized that C2 and C5 are asymmetric, one can see that the energies of HOMO and LUMO for the C5 molecule (HOMO: -5.11 eV, LUMO: -2.76 eV) are obviously lower than that of the molecule C2 (HOMO: -4.67 eV, LUMO: -2.09 eV) and the energy gap between HOMO and LUMO of C5 is also lower than that of C2 with a lower energy gap (2.35 eV). This may be attributed to the presence of electron-attracting NO_2 side groups. On the other hand, the comparison between C2 and C4 show that the replacement of two triple with two double bonds causes a decrease of band gap and a net destabilization of both HOMO and LUMO levels. This is in agreement with what was found in experimental results (Marrocchi et al., 2010).

The calculated band gap E_{gap} of the studied compound increases in the following order: C1 > C4 > C6 > C3 > C2 > C5. Figure 3 shows detailed data of absolute energy of the frontier orbitals for studying compounds, Indium tin oxide (ITO), [6.6]-phenyl-C61-butyric acid methyl ester (PCBM) (substituted C_{60}) and aluminum (Al) is included for comparison purposes. It was deduced that substitution pushes up/down the HOMO/LUMO energies in agreement with their electron acceptor character. To evaluate the possibilities of electron transfer from the excited studied molecules to the conductive band of PCBM, we have studied the photovoltaic properties of the compounds C1 as donor blended with PCBM, which is the most broadly used as an acceptor in solar cell devices. As shown in Table 3, the change of the electron-donor shows a great effect on the HOMO and on the LUMO levels. The experiment phenomenon was quite consistent with previous literature (Derouiche and Djara, 2007; Zhang et al., 2008), which 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 LUMO level of PCBM (open circuit voltage, Voc). The theoretical values of Voc were calculated from the following expression:

$$\mathrm{Voc} = E_{HOMO}\,(\mathrm{Donor}) - \mathrm{E}_{\mathrm{LUMO}}\,(\mathrm{Acceptor}) - 0.3$$

As shown in Figure 3 and knowing that in organic solar cells, the Voc is found to be linearly dependent on the HOMO level of the donor and the LUMO level of the acceptor (Gunes et al., 2007). The calculated Voc of the studied molecules range from 1.14 to 1.58 eV; 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 and the subsequent regeneration is

Table 3. Energy values of E_{LUMO} (ev), E_{HOMO} (ev) and the Voc (ev).

Compound	E_{LUMO} (ev)	E_{HOMO} (ev)	V_{oc} (ev)
C1	-1.488	-4.960	1.434
C2	-2.096	-4.672	1.146
C3	-2.025	-4.806	1.280
C4	-1.820	-4.774	1.248
C5	-2.760	-5.112	1.586
C6	-2.033	-4.939	1.413
PCBM	-3.226	-5.985	-

Table 4. Values of Gap energy (eV) of the several studied compounds in their neutral and doped forms.

Compound	E_{gap} (eV) neutral	E_{gap} (eV) polaronic
C1	3.47	2.87
C2	2.57	2.26
C3	2.78	2.60
C4	2.95	2.35
C5	2.35	2.32
C6	2.90	2.74
C7	2.20	2.01

possible in an organic sensitized solar cell.

On the other hand, and since the p-doped π-conjugated molecule has becomes the ultimate responsible of charged transport, the values of the energy of the HOMO, LUMO, E_{gap} (E_{HOMO} - E_{LUMO}) for several compounds in their neutral and polaronic forms were determinate and shown in Table 4. Available values of the gap energy in neural state are presented also in this table for comparison. Traditionally and until now, charged state in conjugated molecules has been discussed in terms of one-electron band model. We note that the energy gap decreases when passing from the neutral to the doped form for all oligomers.

Finally, it is important to examine the HOMO and the LUMO for these compounds because the relative ordering of occupied and virtual orbital provides a reasonable qualitative indication of excitations properties (Yang et al., 2005). In general, as shown in Figure 4 (LUMO, HOMO), the HOMOs of these oligomers in the neutral form possess a π-bonding character within subunit and a π-anti-bonding character between the consecutive subunits; while the LUMOs possess a π-anti-bonding character within subunit and a π-bonding character between the subunits, whereas it is the opposite in the case of doped forms.

Absorption and electronic properties

Based on the optimized molecular structures with B3LYP/6-31G(d) method, we have calculated the ultraviolet-visible (UV-Vis) spectra of the studied compounds C1, C2, C3, C4, C5 and C6 using ZINDO/s method. As shown in Table 5, we can find the values of calculated wavelength λ_{max} and for comparison experimental ones excitation to the S_1 state corresponds almost exclusively to the promotion of an electron from the HOMO to the LUMO orbital. The absorption wavelengths arising from $S_0 \rightarrow S_1$ electronic transition increase progressively with the increasing of conjugation lengths. It is reasonable, since HOMO→LUMO transition is predominant in $S_0 \rightarrow S_1$ electronic transition; the results are a decrease of the LUMO and an increase of the HOMO energy.

These values are calculated by ZINDO method starting with optimized geometry obtained at B3LYP/6-31G(d) level. However, we believe that the bulk of intermolecular effect must be taken into account. This effect is the source of the deviation between the calculation and the experimental results.

We can remark for comparing calculated and experimental results (Marrocchi et al., 2010) a linear relationship between calculated and experiment results. Therefore, the DFT theoretical calculations give a good description of the absorption properties of the studied compound and can be employed to predict the electronic characteristics of other materials. It should be noted that the difference between theoretical and experimental values can be explained by the fact that the calculations assume that the molecules are in the vapour state.

Another considered point is that the position of λmax shows a bathochromic shift when passing from C1 to C6,

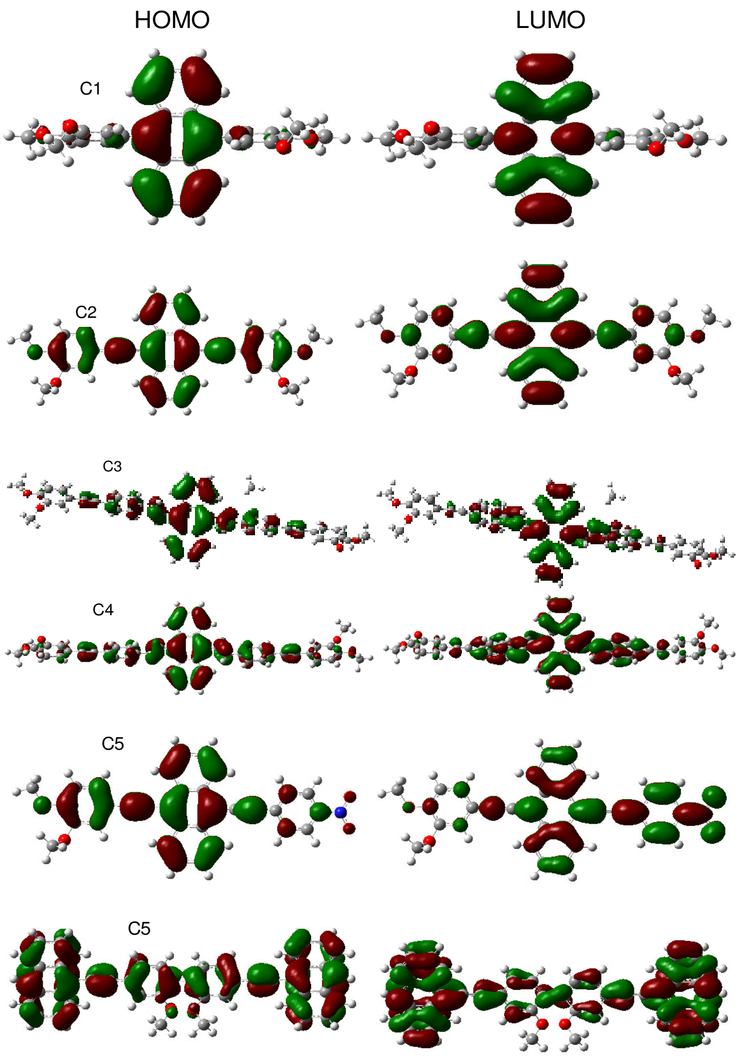

Figure 4. The contour plots of HOMO and LUMO orbitals of study compounds C1 to C6 in neutral form.

which also can be seen, respectively in C1 (397.54 nm), C2 (494.19 nm), C3 (460.17 nm), C4 (447.35 nm), C5 (514.20 nm) and C6 (442.76 nm) due to the increasing of the extended conjugation through the system of aryl groups and multiple bonds. The asymmetrically substituted compounds C5, containing a nitro-group, show absorption spectra red-shifted of about 20 nm with respect to the symmetric analogous to C2 and finally the presence of two anthracene units in C6 does not cause a significant red shift of the absorption. Those interesting points are seen both in the theoretical and experimental results.

Conclusion

In this study, theoretical analysis of the geometries and electronic properties of several various compounds based on the anthrance was performed using the DFT/B3LYP method. The effect of substituted groups on the structural and opto-electronic properties of these materials and the possibility of their application as organic solar cells are discussed. The concluding remarks are:

1) The results of the optimized structures for all studied compounds so that they have similar conformations (quasi planar conformation). We found that the incorporation of several groups does not change the geometric parameters.
2) During the doping process and for all studied compounds the simple bonds become shorter, while the multiple ones become longer. The inter-rings bonds are longer than normal double bonds. A quinoid-like distortion emerges as a result of the oxidation
3) The calculated frontier orbital energies HOMO and

Table 5. Absorption λ_{abs} (nm) obtained by the ZINDO/DFT method.

Compound	λ_{max} (nm) ZINDO	OS	λ_{max} exp (nm)	
			Chloroform	Cyclohexane
C1	397.54	0.4317	398	375, 395
C2	494.49	1.1089	475	478
C3	460.17	1.5308	464	460
C4	447.35	0.9057	418	413
C5	514.20	1.3002	494	492
C6	442.76	1.5183	444	439

LUMO and energy gaps showed that the energy gaps of the studied molecules differ slightly from 2.35 to 3.47 eV depending on the different structures. The calculated band gap E_{gap} of the studied compound increases in the following order C1 > C4 > C6 > C3 > C2 > C5.

4) The replacement of two triple with two double bonds causes a decrease of band gap and a net destabilization of both HOMO and LUMO levels

5) All the studied molecules can be used as sensitizers because the electron injection process from the excited molecule to the conduction band of PCBM and the subsequent regeneration are feasible in the organic 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 application. Presumably, the procedures of theoretical calculations can be employed to predict and assume the electronic properties on yet prepared and efficiency proved other materials, and to further to novel materials for organic solar cells.

ACKNOWLEDGEMENTS

This work was supported by Volubilis Program (N° MA/11/248), and the convention CNRST/CNRS (Project chimie1009). We are grateful to the “Association Marocaine des Chimistes Théoriciens” (AMCT) for its pertinent help concerning the programs

REFERENCES

Becke AD (1993). Density-functional thermochemistry. III. The role of exact exchange J. Chem. Phys. 98:5648-5653.

Bouachrine M, Echchary A, Bouzzine SM, Amine M, Hamidi M, Amine A, Zair T (2011). Oligothiophenes bridged by silicon groups, DFT study of structural and electronic properties. Phys. Chem. News. 58: 61-66.

Bouzakraoui S, Bouzzine SM, Bouachrine M, Hamidi M (2005). Density functional theory study of conformational and opto-electronic properties of oligo-para-phenylenes. J. Mol. Struct. (Theochem). 725:39-44.

Bouzakraoui S, Bouzzine SM, Bouachrine M, Hamidi M (2006). Theoretical investigation of electroluminescent alkoxy substituted 4,4′-bis(2-phenylethenyl)biphenyls as guest in blue OLEDs; Sol. Energy Mater Sol. Cells. 90:1393-1402.

Bouzzine SM, Bouzakraoui S, Bouachrine M, Hamidi M (2005). Density functional theory (B3LYP/6-31G*) study of oligothiophenes in their aromatic and polaronic states. J. Mol. Struct. (Theochem). 726:271-276.

Bouzzine SM, Makayssi A, Hamidi M, Bouachrine M (2008). Bridging effect on structural and optoelectronic properties of oligothiophene. J. Mol. Struct. (Theochem). 851:254-262.

Brabec CJ, Sariciftci NS, Hummelen JC (2001). Plastic Solar Cells. Adv. Funct. Mater. 11: 15-26. Zhou Y, Peng P, Han L, Tian W (2007). Novel donor–acceptor molecules as donors for bulk heterojunction solar cells. Synth. Met. 157: 502-507.

Brocks G, Tol A (1996). Small Band Gap Semiconducting Polymers Made from Dye Molecules:□ Polysquaraines. J. Phys. Chem. 100(5):1838-1846.

Bundgaard E, Krebs FC (2007). Low band gap polymers for organic photovoltaics. Sol. Energy Mater. Sol. Cells 91:954-985.

Casado J, Ramirez FJ, Hotta S, Lopez Navarrete JT, Hernandez V (1997).Vibrational Spectroscopy study of doping induced charged defects in a series of α,α'-Dimethyl end-capped Oligothiophenes. Synth. Met. 84:571-572.

Cornil J, Beljonne D, Brédas JL, Mûllen K, Wegner G (Eds.) (1998). Electronic Materials: The oligomers Approach, Wiley-VCH, Weinheim, New York. pp. 432-447.

Cravino A, Zerza G, Neugebauer H, Maggini M, Bucella S, Menna E, Svensson M, Andersson MR, Brabec CJ, Sariciftci NS (2002). Electrochemical and Photophysical Properties of a Novel Polythiophene with Pendant Fulleropyrrolidine Moieties: Toward “Double Cable” Polymers for Optoelectronic Devices. J. Mater. Chem. 12:1931-1943.

Derouiche H, Djara V (2007). Impact of the energy difference in LUMO and HOMO of the bulk heterojunctions components on the efficiency of organic solar cells. Sol. Energy Mater. Sol. Cells. 91:1163-1167.

Dimitrakopolous CD, Malenfrant PRL (2002). Organic Thin Film Transistors for Large Area Electronics. Adv. Mater. 14:99-117.

Ditchfield R, Hehre WJ, Pople JA (1971). Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules J. Chem. Phys. 54:724-728.

Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JA, Vreven T, Kudin KNJr, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W; Wong MW, Gonzalez C, Pople JA (2003). GAUSSIAN 03, Revision B. 04; Gaussian: Pittsburgh, PA.

Gordon MS (1980). The isomers of silacyclopropane. Chem. Phys. Lett. 76:163-168.

Gunes S, Neugebauer H, Sariciftci NS (2007). Conjugated Polymer-Based Organic Solar Cells. Chem. Rev. 107:1324-1338.

Hariharan PC, Pople JA (1974). Accuracy of AH n equilibrium geometries by single determinant molecular orbital theory. Mol. Phys. 27:209-214.

Hehre WJ, Ditchfiesld R, Pople JA (1972). Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. J. Chem. Phys. 56:2257-2261.

Kim DH, Ohshita J, Lee KH, Kunugi Y, Kunai A (2006). Synthesis of π-Conjugated Oligomers Containing Dithienosilole Units. Organometallics 25:1511-1516.

Kraft A, Grimsdale AC, Holmes AB (1998). Electroluminescent Conjugated Polymers-Seeing Polymers in a New Light. Angew. Chem. Int. Ed. 37:402-428;

Lim E, Jung BJ, Shim HK, Taguchi T, Noda B, Kambayashi T, Mori T, Ishikawa K, Takezoe H, Do LM (2006). Nanoscale thin-film morphologies and field-effect transistor behavior of oligothiophene derivatives. Org. Electron. 7:121-31.

Manoj AG, Narayan KS (2003). Photovoltaic properties of polymer p-n junctions made with P3OT/BBL bilayers. Opt. Mater. 21:417-420.

Marrocchi A, Spalletti A, Ciorba S, Seri M, Elisei F, Taticchi A (2010). Synthesis and photophysical properties of conjugated anthracene-based compounds. J. Photochem. Photobiol. A: Chem. 211:162-169.

Meille SV, Farina A, Bezziccheri F and Gallazi MC (1994). Green Electroluminescence in Poly-(3-cyclohexylthiophene) light-emitting diodes. Adv. Mater. 6:488-490.

Mondal R, Becerril HA, Verploegen E, Kim D, Norton JE, Miyaki SKo, Lee S, Toney MF, Bredas JL, McGehee MD, Bao Z (2010). Thiophene-rich fused-aromatic thienopyrazine acceptor for donor–acceptor low band-gap polymers for OTFT and polymer solar cell applications. J. Mater. Chem. 20:5823-5834.

Müllen K, Wegner G (Eds) (1998). Electronic Materials: The oligomers Approach, Wiley-VCH, Weinheim, New York. pp. 105-197.

Nalwa HS, Ed. John Wiley and Sons (1999). Handbook of Organic Conductive Molecules and Polymers.

Roquet S, Cravino A, Leriche P, Aleveque O, Frere P, Roncali J (2006). Triphenylamine−Thienylenevinylene Hybrid Systems with Internal Charge Transfer as Donor Materials for Heterojunction Solar Cells. J. Am. Chem. Soc. 128:3459-3466.

Sariciftci NS, Smilowitz L, Heeger AJ, Wudl F (1992). Photoinduced electron-transfer from a conducting polymer to Buckminster fullerene. Science. 258:1474-1476.

Wienk MM, Kroon JM, Verhees WJH, Knol J, Hummelen JC, Van Hal PA (2003). Janssen RA. Angew. Chem. Int. Ed. 42:3371-3375.

Yang L, Feng J, Ren A (2005). Theoretical studies on the electronic and optical properties of two thiophene–fluorene based π-conjugated copolymers. Polymer. 46:10970-10981.

Zgou H, Bouzzine SM, Bouzakraoui S, Hamidi M, Bouachrine M (2008). Theoretical study of structural and electronic properties of oligo(thiophene-phenylene)s in comparison with oligothiophenes and oligophenylenes. Chin. Chem. Lett. 19:123-126.

Zhang L, Zhang Q, Ren H, Yan H, Zhang J, Zhang H, Gu J (2008). Calculation of band gap in long alkyl-substituted heterocyclic-thiophene-conjugated polymers with electron donor–acceptor fragment. Sol. Energy Mater. Sol. Cells. 92:581-587.