

Scholars Research Library (http://scholarsresearchlibrary.com/archive.html)



# Theoretical analysis and electronic structure of conjugated systems based on pyrrole. Photovoltaic properties and opto-electronic applications

T. Abram<sup>1</sup>, A. Adad<sup>2</sup>, L. Bejjit<sup>1</sup>, M. Bouachrine<sup>1</sup> and T. Lakhlifi<sup>2</sup>\*

<sup>1</sup>MEM, High School of Technology (ESTM), University Moulay Ismail, Meknes, Morocco <sup>2</sup>Molecular Chemistry and Natural Substances Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco

### ABSTRACT

In this paper, a theoretical study of several conjugated aromatic compounds based on several pyrroleis reported using Density Functional Theory method (DFT). Theoretical calculation has been carried out in order to characterize their stability, geometric and electronic properties. In fact, substituent nature, number and position are crucial parameters to define structural and electronic molecule properties. Besides, assessing HOMO and LUMO energy levels of compounds is essential in investigating suitable materials for optoelectronic applications. The theoretical knowledge of HOMO and LUMO energy levels of the components are basic in studying organic solar cells, so the HOMO, LUMO and Gap energy Voc (open circuit voltage) of the studied compounds have been calculated and discussed. The properties suggest these materials as a good candidate for organic solar cells.

**Keywords:**  $\pi$ -conjugated molecules, pyrrolederivatives, DFT, band-gap, electronic properties, Voc(open circuit voltage).

### INTRODUCTION

Organic materials based on conjugated molecules have attracted continuing interest as a result of their suitability in a broad range of electronic applications, such a batteries [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 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]. Moreover, the short conjugated molecules units have attracted much attention, because of their unique electronic properties, to their high photoluminescence quantum efficiency and thermal stability [7]. Many studies have been made recently on the integration of conjugated heterocyclic and the effect on the optoelectronic properties [8]. Previously [1] have described the synthesis of a series of 3,4-dihydro 2H-pyrrole (Figure 1). To the best of our knowledge a systematic theoretical study of such compounds has not been reported. Fundamental understanding of structural and energetic properties of this kind of materials could be useful so as design new molecules.

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  $\pi$ -conjugated compounds have given great contributions to the rationalization of the properties of known materials and to the prediction of the yet unknown ones. In this context, quantum chemical methods have been increasingly applied to predict the band gap of conjugated systems [9]. This work will further elucidate geometric and electronic properties with the aim to prove the relationship between molecular structure and electronic properties, and driving towards

the next synthesis compounds which are as active materials in optoelectronic. The quantum chemical investigation has been performed to the optical and electronic properties of a series of compounds based on 3,4-dihydro 2H-pyrrole, 2H-pyrrole and pyrrole derivatives. 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 basis in studying organic solar cells as the HOMO, LUMO, Gap energy and Voc of the studied compounds have been calculated and reported. Particular attention is paid to electronic structure, absorption and emission properties. Their properties suggest they are good candidates for organic solar cells.



Figure 1: Chemical structure of studied compounds Pyr<sub>i</sub> (I = 1–26)

### MATERIALS AND METHODS

DFT method of three-parameter compound of Becke (B3LYP) [10] was used in all the study of the neutral and polaronic compounds. The 6-31G (d) basis set was used for all calculations [11]. 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 [12]. The geometry structures of neutral molecules were optimized under no constraint. We have also examined HOMO and LUMO levels; the energy  $E_{gap}$  is evaluated as 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 [13].

#### RESULTS

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 ring does not change the geometric parameters.





Table 1 lists the calculated frontier orbital energies and energy  $E_{gap}$  between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and the energyEgap of the studied molecules, also the open circuit voltageV<sub>oc</sub>(eV) and  $= E_{LOMO}$  (Donor)  $-E_{LUMO}$  (Acceptor). These parameters will be discussed in the photovoltaic part.

Table 1: Energy values of  $E_{LUMO}$  (eV),  $E_{HOMO}$  (eV),  $E_{gap}$  (eV),  $\alpha$  (eV) and the open circuit voltage  $V_{oc}$  (eV) of the studied molecules obtained by B3LYP/6-31G (d)

N°	E <sub>HOMO</sub> (eV)	E <sub>LUMO</sub> (eV)	Egap (eV)	Voc(eV)	a (eV)
Pyr <sub>1</sub>	-6.081	-2.023	4.058	2.081	1.677
Pyr <sub>2</sub>	-5.558	-2.351	3.207	1.558	1.349
Pyr <sub>3</sub>	-5.491	-2.332	3.159	1.491	1.368
Pyr <sub>4</sub>	-5.625	-2.404	3.221	1.625	1.296
Pyr <sub>5</sub>	-5.514	-2.355	3.159	1.514	1.345
Pyr <sub>6</sub>	-5.503	-2.576	2.927	1.503	1.124
Pyr <sub>7</sub>	-5.543	-2.610	2.933	1.543	1.090
Pyr <sub>8</sub>	-5.475	-2.327	3.148	1.475	1.373
Pyr <sub>9</sub>	-5.539	-2.321	3.218	1.539	1.379
Pyr <sub>10</sub>	-5.684	-1.892	3.792	1.684	1.808
Pyr <sub>11</sub>	-5.683	-1.869	3.815	1.683	1.831
Pyr <sub>12</sub>	-5.475	-1.727	3.748	1.475	1.973
Pyr <sub>13</sub>	-5.514	-1.683	3.831	1.514	2.017
Pyr <sub>14</sub>	-5.706	-1.856	3.849	1.706	1.844
Pyr <sub>15</sub>	-5.513	-1.732	3.781	1.513	1.968
Pyr <sub>16</sub>	-5.494	-1.805	3.689	1.494	1.895
Pyr <sub>17</sub>	-5.430	-2.255	3.176	1.430	1.445
Pyr <sub>18</sub>	-5.902	-1.895	4.007	1.902	1.805
Pyr <sub>19</sub>	-5.634	-1.691	3.943	1.634	2.009
Pyr <sub>20</sub>	-5.978	-1.940	4.038	1.978	1.760
Pyr <sub>21</sub>	-5.764	-1.760	4.003	1.764	1.940
Pyr <sub>22</sub>	-5.753	-1.816	3.937	1.753	1.884
Pyr <sub>23</sub>	-5.962	-1.957	4.005	1.962	1.743
Pyr <sub>24</sub>	-5.966	-1.919	4.047	1.966	1.781
Pyr <sub>25</sub>	-5.787	-1.815	3.972	1.787	1.885
Pyr <sub>26</sub>	-5.626	-1.949	3.677	1.626	1.751
PCBM C <sub>60</sub> (A)	-6.100	-3.700	-	-	-

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 Pyr<sub>1</sub> to Pyr<sub>26</sub> change significantly, the LUMOs for Pyr<sub>1</sub>, Pyr<sub>2</sub>, Pyr<sub>3</sub>, Pyr<sub>4</sub>, Pyr<sub>5</sub>, Pyr<sub>6</sub>, Pyr<sub>7</sub>, Pyr<sub>8</sub>, Pyr<sub>9</sub>, Pyr<sub>10</sub>, Pyr<sub>11</sub>, Pyr<sub>12</sub>, Pyr<sub>13</sub>, Pyr<sub>14</sub>, Pyr<sub>15</sub>, Pyr<sub>16</sub>, Pyr<sub>17</sub>, Pyr<sub>18</sub>, Pyr<sub>19</sub>, Pyr<sub>20</sub>, Pyr<sub>21</sub>, Pyr<sub>22</sub>, Pyr<sub>23</sub>, Pyr<sub>24</sub>, Pyr<sub>25</sub> and Pyr<sub>26</sub> are located at -2.023; -2.351; -2.332; -2.404; -2.355; -2.576; -2.610; -2.327; -2.321; -1.892; -1.8669; -1.727; -1.683; -1.856; -1.732; -1.805; -2.255; -1.895; -1.691; -1.940; -1.760; -1.816; -1.957; -1.919; -1.815 and -1.949 eV, respectively. The HOMOs for Pyr<sub>1</sub>, Pyr<sub>2</sub>, Pyr<sub>3</sub>, Pyr<sub>4</sub>, Pyr<sub>5</sub>, Pyr<sub>6</sub>, Pyr<sub>7</sub>, Pyr<sub>8</sub>, Pyr<sub>9</sub>, Pyr<sub>10</sub>, Pyr<sub>11</sub>, Pyr<sub>12</sub>, Pyr<sub>13</sub>, Pyr<sub>14</sub>, Pyr<sub>15</sub>, Pyr<sub>16</sub>, Pyr<sub>17</sub>, Pyr<sub>18</sub>, Pyr<sub>19</sub>, Pyr<sub>20</sub>, Pyr<sub>21</sub>, Pyr<sub>22</sub>, Pyr<sub>23</sub>, Pyr<sub>24</sub>, Pyr<sub>25</sub> and Pyr<sub>26</sub> are located at -6.081; -5.558; -5.491; -5.625; -5.514; -5.503; -5.543; -5.475; -5.539; -5.684; -5.683; -5.475; -5.514; -5.706; -5.513; -5.494; -5.494; -5.430; -5.902; -5.634; -5.978; -5.764; -5.753; -5.962; -5.966; -5.787 and -5.626 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 ( $E_{gap}$ ) of the studied molecules differs slightly from 2.927 eVto 4.058 eV depending on the different structures. They are studied in the following order:

## $\begin{array}{l} Pyr_{1} > Pyr_{24} > Pyr_{20} > Pyr_{18} > Pyr_{23} > Pyr_{21} > Pyr_{25} > Pyr_{19} > Pyr_{22} > Pyr_{14} > Pyr_{13} > Pyr_{10} > Pyr_{10} > Pyr_{15} > Pyr_{16} > Pyr_{26} > Pyr_{4} > Pyr_{9} > Pyr_{2} > Pyr_{17} > Pyr_{3} > Pyr_{5} > Pyr_{8} > Pyr_{7} > Pyr_{6} \end{array}$

Generally, the most efficient material solar cells are based on the bulk hetero-junction structure of the blend of  $\pi$ -conjugated molecule or polymer donors and fullerene derivative acceptors [14]. Here, we have studied the photovoltaic properties of the compounds Pyr<sub>1</sub> to Pyr<sub>26</sub> as donor blended with [6.6]-phenyl-C<sub>61</sub>-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 3 shows detailed data of absolute energy of the frontier orbitals for studying compounds and PCBM as an acceptor. 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. As shown in Table 1, both HOMO and LUMO levels of the studied molecules agreed well with the requirement for an efficient photosentizer. Indeed, the difference in the LUMO energy levels of the studied compounds Pyr<sub>1</sub> to Pyr<sub>26</sub> and PCBM was in the range of 1,090 to 2,017 eV, suggesting that the photo-excited electron transfer from our compounds to PCBM may be sufficiently efficient to be useful in photovoltaic devices [15].

On the other hand and 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 [16]. The power conversion efficiency (PCE) was calculated according to the following equation (1):

$$PCE = \frac{1}{P_{in}(FF. V_{oc}. J_{sc})}$$
(1)

Where  $P_{in}$  is the incident power density,  $J_{sc}$  is the short-circuit current,  $V_{oc}$  is the open-circuit voltage, and FF denotes the fill factor. The maximum open circuit voltage ( $V_{oc}$ ) of the Bulk Hetero Junction solar cell is related to the difference between the highest occupied molecular orbital (HOMO) of the electron donor and the LUMO of the electron acceptor, taking into account the energy lost during the photo-charge generation [17]. The theoretical values of open-circuit voltage  $V_{oc}$  have been calculated from the following expression (2):

$$\mathbf{V}_{oc} = \left| \mathbf{E}_{HOMO} \left( \mathbf{Donor} \right) \right| - \left| \mathbf{E}_{LUMO} \left( \mathbf{Acceptor} \right) \right| - 0.3$$
 (2)

The obtained values of  $V_{oc}$  of the studied molecules range from 1,430 eV to 2,081 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 fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) and the subsequent regeneration is possible in an organic sensitized solar cell (Table 1, Figure 3).



Figure 3:Sketch of DFT/B3LYP/6-31G (d) calculated energy of the HOMO, LUMO levels of studied molecules

The frontier molecular orbital (MO) contribution is very important in determining the charge-separated states of the studied molecules because the relative ordering of occupied and virtual orbital provides a reasonable qualitative indication of excitations properties [18]. In general, as shown in figure 4 (LUMO, HOMO), the HOMOs of these oligomers in the neutral form possess a  $\pi$ -bonding character within subunit and a  $\pi$ -antibonding character between the consecutive subunits while the LUMOs possess a  $\pi$ -antibonding character within subunit and a  $\pi$ -bonding character between the subunits whereas it is the opposite in the case of doped forms.









Figure 4: Obtained isodensity plots of the frontier orbital HOMO and LUMO of the studied compounds obtained at B3LYP/6-31(d) level

Absorption Properties based on the optimized molecular structures with B3LYP/6-31G (d) method. We have calculated the UV-vis. spectra of each studied compound:  $Pyr_i$  (1 to 26) using by ZINDO method (Figure 5).

As illustrated in table 2, we can find the values of calculated wavelength  $\lambda_{abs}$  and oscillator strengths O.S. Excitation to the S<sub>1</sub> state corresponds almost exclusively to the promotion of an electron from the HOMO to the LUMO orbital. The absorption wavelengths arising from S<sub>0</sub> $\rightarrow$ S<sub>1</sub> electronic transition increase progressively with the

increasing of conjugation lengths. It is reasonable, since HOMO $\rightarrow$ LUMO transition is predominant in S<sub>0</sub> $\rightarrow$ S<sub>1</sub> electronic transition; the results are a decrease of the LUMO and an increase of the HOMO energy [19].

These values are calculated by ZINDO method starting with optimized geometry obtained at B3LYP/6-31G (d) level. Data in table 5 shows that there is a bathochromic shift when passing from Pyr<sub>1</sub> to Pyr<sub>26</sub> in this order (Pyr<sub>1</sub>, Pyr<sub>2</sub>, Pyr<sub>3</sub>, Pyr<sub>4</sub>, Pyr<sub>5</sub>, Pyr<sub>6</sub>, Pyr<sub>7</sub>, Pyr<sub>8</sub>, Pyr<sub>9</sub>, Pyr<sub>10</sub>, Pyr<sub>11</sub>, Pyr<sub>12</sub>, Pyr<sub>13</sub>, Pyr<sub>14</sub>, Pyr<sub>15</sub>, Pyr<sub>16</sub>, Pyr<sub>17</sub>, Pyr<sub>18</sub>, Pyr<sub>19</sub>, Pyr<sub>20</sub>, Pyr<sub>21</sub>, Pyr<sub>22</sub>, Pyr<sub>23</sub>, Pyr<sub>24</sub>, Pyr<sub>25</sub>, Pyr<sub>26</sub>) which also can be seen respectively in Pyr<sub>1</sub> (356.13nm), Pyr<sub>2</sub> (374.09nm), Pyr<sub>3</sub> (362.26nm), Pyr<sub>4</sub> (374.02nm), Pyr<sub>5</sub> (357.84nm), Pyr<sub>6</sub> (376.09nm), Pyr<sub>7</sub> (371.13nm), Pyr<sub>8</sub> (374.17nm), Pyr<sub>9</sub> (352.43nm), Pyr<sub>10</sub> (317.58nm), Pyr<sub>11</sub> (333.19nm), Pyr<sub>12</sub> (326.97nm), Pyr<sub>13</sub> (319.99nm), Pyr<sub>14</sub> (341.93nm), Pyr<sub>15</sub> (299.51nm), Pyr<sub>16</sub> (332.33nm), Pyr<sub>17</sub> (361.63nm), Pyr<sub>18</sub> (303.10nm), Pyr<sub>19</sub> (312.71nm), Pyr<sub>20</sub> (330.91nm), Pyr<sub>21</sub> (308.32nm), Pyr<sub>22</sub> (311.36nm), Pyr<sub>23</sub> (321.41nm) , Pyr<sub>24</sub> (339.02nm), Pyr<sub>25</sub> (332.82nm), Pyr<sub>26</sub> (320.52nm). This effect is obviously due to insertion of different Donor or acceptor to the  $\pi$ -spacer unit. Those interesting points are seen both in the theoretical and experimental results.

Table 2: Absorption spectra data obtained by ZINDOmethods for the Pyr <sub>i</sub> (i=1 to 26) compounds at B3LYP/6-31G (d) optimized
geometries

N°	λ (nm)	Eactivation	<b>0.</b> S	MO/character
Pyr <sub>1</sub>	356.13	3.4815	0.7189	HOMO→LUMO (94%)
Pyr <sub>2</sub>	374.09	3.3143	0.4789	HOMO→LUMO (92%)
Pyr <sub>3</sub>	362.26	3.4225	0.6699	HOMO→LUMO (94%)
Pyr <sub>4</sub>	374.02	3.3149	0.4418	HOMO→LUMO (90%)
Pyr5	357.84	3.4648	0.6877	HOMO→LUMO (94%)
Pyr <sub>6</sub>	376.09	3.2967	0.4055	HOMO→LUMO (86%)
Pyr <sub>7</sub>	371.13	3.3408	0.4624	HOMO→LUMO (87%)
Pyr <sub>8</sub>	374.17	3.3135	0.4690	HOMO→LUMO (92%)
Pyr <sub>9</sub>	352.43	3.5180	0.1283	HOMO-1→LUMO (86%)
Pyr <sub>10</sub>	317.58	3.9039	0.4555	HOMO→LUMO (95%)
Pyr <sub>11</sub>	333.19	3.7210	0.4045	HOMO→LUMO (89%)
Pyr <sub>12</sub>	326.97	3.7917	0.4265	HOMO→LUMO (95%)
Pyr <sub>13</sub>	319.99	3.8744	0.4457	HOMO→LUMO (95%)
Pyr <sub>14</sub>	341.93	3.6258	0.2127	HOMO-1→LUMO (22%)
Pyr <sub>15</sub>	299.51	4.1394	0.3478	HOMO-1→LUMO (86%)
Pyr <sub>16</sub>	332.33	3.7306	0.3908	HOMO→LUMO (88%)
Pyr <sub>17</sub>	361.63	3.4285	0.6585	HOMO→LUMO (94%)
Pyr <sub>18</sub>	303.10	4.0903	0.4274	HOMO→LUMO (95%)
Pyr <sub>19</sub>	312.71	3.9647	0.3979	HOMO→LUMO (94%)
Pyr <sub>20</sub>	330.91	3.7466	0.3318	HOMO-1→LUMO (85%)
Pyr <sub>21</sub>	308.32	4.0211	0.4294	HOMO→LUMO (95%)
Pyr <sub>22</sub>	311.36	3.9818	0.3896	HOMO→LUMO (95%)
Pyr <sub>23</sub>	321.41	3.8573	0.3239	HOMO→LUMO (85%)
Pyr <sub>24</sub>	339.02	3.6570	0.4417	HOMO→LUMO (88%)
Pyr <sub>25</sub>	332.82	3.7251	0.3714	HOMO→LUMO (84%)
Pyr <sub>26</sub>	320.52	3.8680	0.3205	HOMO→LUMO (82%)

Data in table 2 shows that there is a bathochromic shift when passing from  $Pyr_6$  (376.09nm) to  $Pyr_{15}$  (299.51nm). This effect is obviously due to the aromaticity in the studied compounds. Those interesting points are seen both in the studying the electronic and absorption properties.

The calculated wavelength  $\lambda_{abs}$  of the studied compounds decreases in the following order:

# $\begin{array}{l} Pyr_6 > Pyr_8 > Pyr_2 > Pyr_4 > Pyr_7 > Pyr_3 > Pyr_{17} > Pyr_5 > Pyr_1 > Pyr_9 > Pyr_{14} > Pyr_{24} > Pyr_{11} > Pyr_{25} > Pyr_{16} > Pyr_{20} > Pyr_{12} > Pyr_{23} > Pyr_{26} > Pyr_{13} > Pyr_{10} > Pyr_{19} > Pyr_{22} > Pyr_{21} > Pyr_{18} > Pyr_{15} \end{array}$

which is the same order of the reduction of the acceptor strength. This bathochromic effect from  $P_i$  is obviously due to increased  $\pi$  delocalization. This interesting point is seen both by analysing electronic and absorption results. Excitation to the S<sub>1</sub>statecorresponds exclusively to the promotion of an electron from the HOMO to the LUMO. The absorption wavelengths arising from S<sub>0</sub>-S<sub>1</sub>electronic transition increase progressively with the increasing of conjugation lengths. It is reasonable, since HOMO-LUMO transition is predominant in S<sub>0</sub>-S<sub>1</sub>electronic transition; the results are a decrease of the LUMO and an increase of the HOMO energy.



Figure 5:Simulated UV-visible optical absorption spectra of title compounds with calculated data at the ZINDO /B3LYP/6-31G (d)

### CONCLUSION

This study is a theoretical analysis of the geometries and electronic properties of three various compounds based on the pyrroles which displays the effect of substituted groups on the structural and opto-electronic 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 all studied compounds so that they have similar conformations (quasi planar conformation). We found that the modification of several groups does not change the geometric parameters. \* The calculated frontier orbital energies HOMO and LUMO and energy  $E_{gap}$  showed that the energy  $E_{gap}$  of the studied molecules differ slightly from 4.058 eV to 2.927 eV depending on the different structures. Also we can remark that the energy  $E_{gap}$  decreases, this is probably due to the effect of the conjugated system and aromaticity in the compounds studied.

\* The energy  $E_{gap}$  of Pyr<sub>6</sub> is much smaller than that of the other compounds.

\* The Molecule  $Pyr_6$  witch have a relatively high value of  $\lambda_{max}$  (absorption), is expected to have the most outstanding photophysical properties.

\*All the studied molecules can be used as BHJ solar cell because the electron injection process from the studied molecule to the conduction band of PCBM and the subsequent regeneration are possible.

\* 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.

### ACKNOWLEDGMENT

This work was supported by Volubilis Program (N° MA/11/248)). We are grateful to the "Association Marocaine des ChimistesThéoriciens" (AMCT) for its pertinent help concerning the programs.

#### REFERENCES

[1]M Birouk; S Harraga; J Panouse-Perrin; J-F Robert; M Damelincourt; F Theobald; R Mercier; J-J Panouse, *Eur. J. Med. Chem.*, **1991**, 26, 91-99.

### Available online at www.scholarsresearchlibrary.com

[2]Ki-Soo Kim; SeonjuJeong; Cham Kim; Jae-Yong Ham; Younghwan Kwon; Byoung-Dae Choi; Yoon Soo Han, *Synthetic Metals.*, **2009**, 159, 1870-1875.

[3]D Tomkute-Luksiene; J Keruckas; T Malinauskas; J Simokaitiene; V Getautis; J V Grazulevicius; D Volyniuk; V Cherpak; P Stakhira; V Yashchuk; V Kosach; G Luka; J Sidaravicius, *Dyes and Pigments*, **2013**, 96, 278-286.

[4]M Kraus; S Haug; W Brütting; A Opitz, Organic Electronics, 2011, 12, 731-735.

[5] Matthew Wright; Ashrafuddin, Solar Energy Materials & Solar Cells, 2012, 107, 87-111.

[6]Y Lei; Q Niu; H Mi; Y Wang; I Nurulla; W Shi, Dyes and Pigments, 2013, 96, 138-147.

[7]P Morvillo; E Bobeico, Solar Energy Materials & Solar Cells, 2008, 92, 1192-1198.

[8]L ChristosChochos; A SteliosChoulis, Progr. Polymer Sci., 2011, 36, 1326-1414.

[9]A IdrissiTaghki , M Bouachrine; M Hnach , S Harraga , J-P-Perrin , B Laude; TLakhlifi, J. Mater. Environ. Sci., 2010, 1 (1), 44-51.

[10]C Lee; W Yang; R G Parr, Physical Review B., 1988, 37, 785-789.

[11]a) A D Becke, Chem. Phys., 1993, 98, 5648-5652.

(b) S H Vosko; L Wilk; M Nusair, *Canadian J. Phys.*, **1980**, 58, 1200-1211.

[12]M J Frisch; G W Trucks; H B Schlegel; G E Scuseria; M A Robb; J R Cheeseman; J A Montgomery; T Vreven; K N JrKudin; J C Burant; J M Millam; S Slyengar; J Tomasi; V Barone; B Mennucci; M Cossi; G Scalmani; N Rega; G A Petersson; H Nakatsuji; M Hada; M Ehara; K Toyota; R Fukuda; J Hasegawa; M Ishida; T Nakajima; Y Honda; O Kitao; H Nakai; M Klene; X Li; J E Knox; H P Hratchian; J B Cross; C Adamo; J Jaramillo; R Gomperts; R E Stratmann; O Yazyev; A J Austin; R Cammi; C Pomelli; J W Ochterski; P Y Ayala; K Morokuma; G A Voth; P Salvador; J JDannenberg; V G Zakrzewski; S Dapprich; A D Daniels; M C Strain; O Farkas; D K Malick; A D Rabuck; K Raghavachari; J B Foresman; J V Ortiz; Q Cui; A G Baboul; S Clifford; J Cioslowski; B BStefanov; G Liu; A Liashenko; P Piskorz; I Komaromi; R L Martin; D J Fox; T Keith; M A Al- Laham; C Y Peng; A Nanayakkara; M Challacombe; P M W Gill; B Johnson; W Chen; M W Wong; C Gonzalez; J A Pople, GAUSSIAN 03, Revision B.04, Gaussian, Inc. Pittsburgh PA. **2003**.

[13]S V Meille; A Farina; F Bezziccheri and M C Gallazi, J. Adv. Mater., 1994, 6, 848-851.

[14]L Zhang; Q Zhang; H Ren; H Yan; J Zhang; H Zhang; J Gu, J. Solar Energy Materials & Solar Cells, 2007, 92, 581-587.

[15]S Gunes; H Neugebauer; N S Sariciftci, J. Chem. Rev., 2006, 107, 1324-1338.

[16]Y J He; H Chen; J H Hou; Y F Li, J. Am. Chem. Soc., **2010**, 132, 1377-1382.

[17](a) A Gadisa; M Svensson; M R Anderson; O Inganas, J. Appl. Phys. Lett., 2004, 84, 1609-1611.

(b) C J Brabec, A Cravino; D Meissner; N S Sariciftci; T Fromherz; M T Rispens; L Sanchez; J C Hummelen, J. Adv. Funct. Mater., **2001**, 11, 374-380.

[18]He-ping Shi; Jian-xin Dai; Li-wen Shi; Lei Xu; Zhao-bin Zhou; Yan Zhang; Wen Zhou; Chuan Dong, *SpectrochimicaActa Part.*, **2012**, 93, 19-25.

[19]T Abram; R Hmamouchi; T Lakhlifi; L Bejjit; M Hamidi; M Bouachrine, J. Mater. Environ. Sci., 2014, 5 (4),1224-1237.