

Novel π -conjugated molecules based on Ethylcarbazol and different acceptor for organic photovoltaic cells. Theoretical investigations

Fatima Agda^{1,2}, Mustafa Taleb¹, Mohamed Benrraou², Mohammed Bouachrine^{3*}

¹LIMME, Faculté des Sciences Dhar Mahraz, Université Sidi Mohammed Ben Abdellah, Fes, Morocco.

²Faculty of Sciences and Technics Errachidia, University Moulay Ismail, Meknes, Morocco

³ESTM, University Moulay Ismail, Meknes, Morocco.

Abstract

In this paper and in order to guide the synthesis of novel materials based on conjugated molecules for optoelectronic applications, we use the DFT method for study of six conjugated compound based on 1,3,5, tris(2-(ethylcarbazyl-3)-ethylene)benzene namely TECEB. The theoretical knowledge of the HOMO and LUMO energy levels of the components is basic in studying organic solar cells. As a result the HOMO, LUMO and Gap energy of the studied compounds have been calculated and reported. The absorption properties were determined by TD/DFT-B3LYP/6-31G calculation. Additionally, several physic-chemical parameters such as inter-ring bond lengths and dihedral angle, E_{gap} , V_{oc} ... were determined from the fully optimized structures. These properties suggest these materials as a good candidate for organic solar cell.

Keywords: derive of ethylcarbazyl, donor, acceptor, TD/DFT-B3LYP, E_{gap} .

1. Introduction

These compounds based on conjugated molecules have become the most promising materials for the optoelectronic device technology [1] such as LEDs [2], Transistors (TFTs) [3] and solar cells [4]. The properties of these materials strongly depend on the degree of electronic delocalisation and effective conjugation length. In recent times a lot of

researchers have become concerned in synthesizing short-chain OLED molecules based on conjugated molecules [5]. These compounds suggest advantages over polymeric systems in terms of easy synthesis and generally exhibit high charge carrier mobility. - More the short conjugated molecules units have attracted much attention because of their unique electronic properties and thermal stability [6]. Recently small organic molecules based on low band gap chromophore began to have great interest as donors in this kind of devices. Indeed, recent work has demonstrated that it is possible to solution process BHJs comprising small organic molecules donor and acceptor phases that are able to achieve power conversion efficiencies (PCEs) comparable to some of the best known polymer systems. In this modest work, we were interested of six novel compounds based on 1, 3, 5, tris (2-(ethylcarbazyl-3)-ethylene) benzene (TECEB), this material was prepared and characterized by LI Jiuyan et al [7]. It's already used as LED. These six compounds M1, M2, M3, M4, M5 and M6 are shown in Fig 1. The geometric, electronic properties, absorption spectra of these studied compounds are studied by using density functional theory (DFT) and time-dependent density functional theory (TD/DFT). The theoretical knowledge of the HOMO and LUMO energy levels of the components is a basis in studying organic solar cells. Consequently, the HOMO, LUMO and Gap energy of the studied compounds have been calculated and reported.

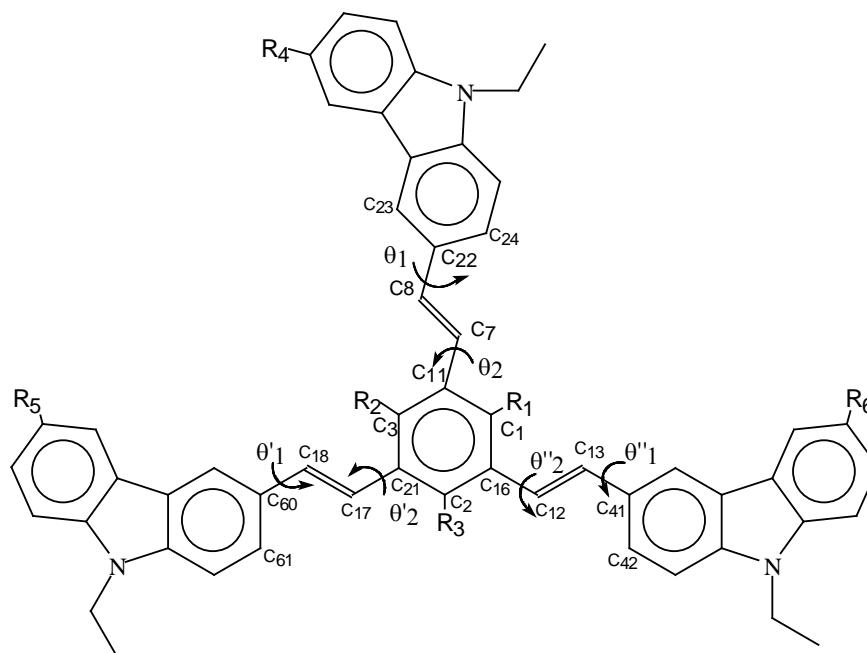


Fig. 1 Molecular structure of the studied compounds (Ri=Br (M1), Ri=Cl (M2), Ri=CN (M3), Ri= COOH (M4), Ri=OCH₃ (M5), Ri=SCH₃ (M6))

2. Materials and methods

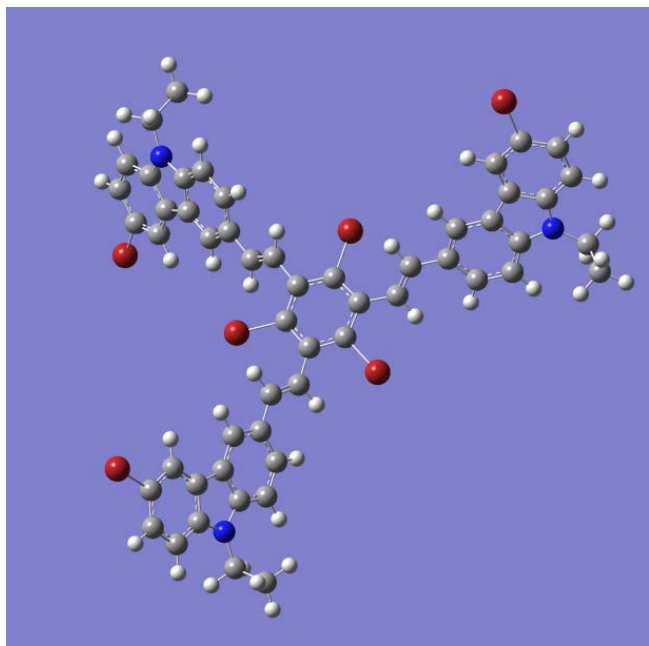
For the geometry optimizations at ground were performed under no constraints in the framework of the DFT methods. These methods have become very popular in recent years because they can reach similar precision to other methods in less time and less cost from the computational point of view. Using the B3LYP functional Becke's three-parameter functional (B3) and includes a mixture of HF with DFT exchange terms associated with the gradient corrected correlation functional of Lee, Yang and Parr (LYP) exchange correlation functional [8]. The 6-31G (d,p) basis set was used for all calculations, and was chosen as a compromise between the quality of the theoretical approach and the high computational cost associated with the high number of dimensions to the problem for all atoms [9]. All computations of the studied molecules in this work were carried out with the Gaussian 03 program package [10] on an Intel Pentium IV 3.3 GHz PC running Linux. The 3D structures of the molecules were generated using the Gauss View software program (version 5.0.8) and the graphical molecular orbital. The HOMO, LUMO and gap's energies were also deduced from the stable structure of the neutral form, where the energy E_{gap} is evaluated as the difference between LUMO and HOMO energies. In

this paper, the transition energies were calculated at the ground-state geometries using TD-DFT/DFT method [11] calculations on the fully optimized geometries. The results obtained gave us the absorption, their corresponding transition energies, and the factor oscillation.

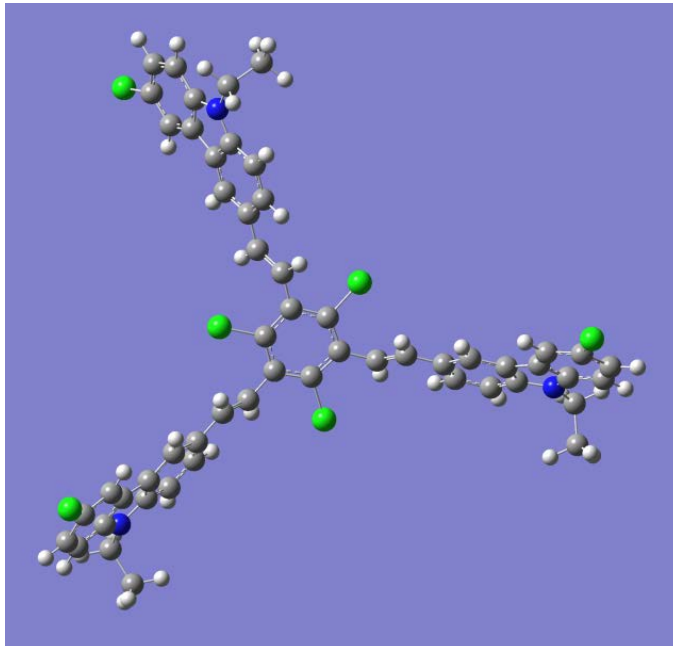
3. Results and discussion

3.1 Molecular design and geometry structure

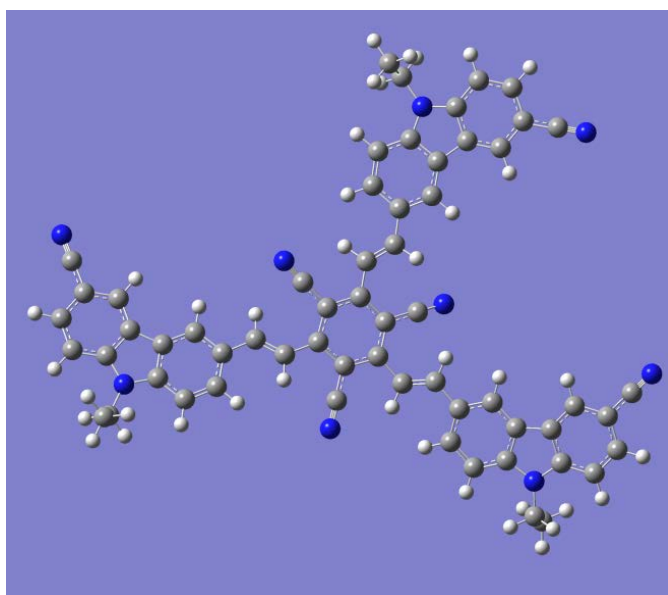
The optimized geometries obtained by B3LYP/6-31G (d, p) of the studied molecules (M1, M2, M3, M4, M5 and M6) are plotted in fig 2. In order to determine the geometrical parameters (inter-ring bond lengths (d_i) and dihedral angles (θ_i)), the molecules are fully optimized in their ground using the 6-31G(d,p) basis set



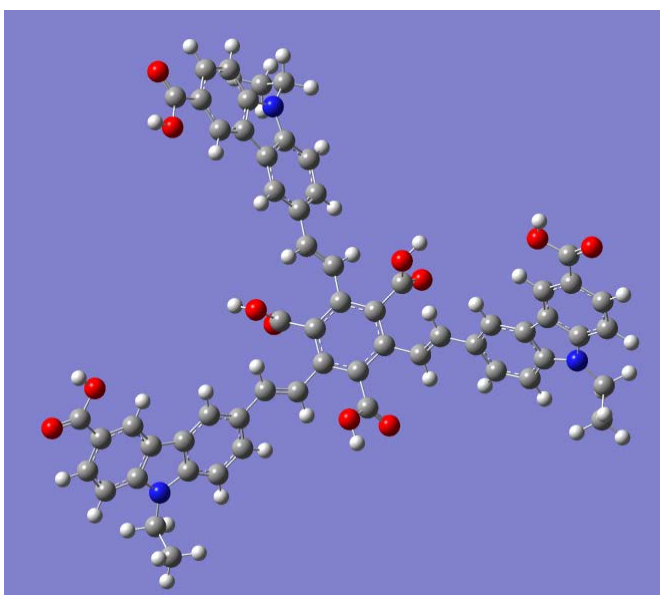
M1



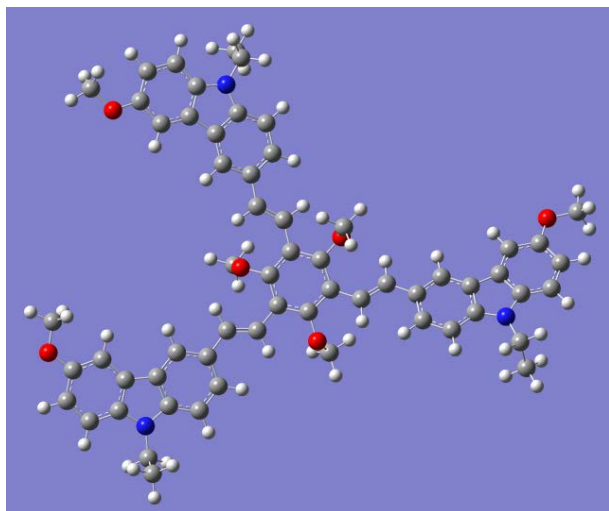
M2



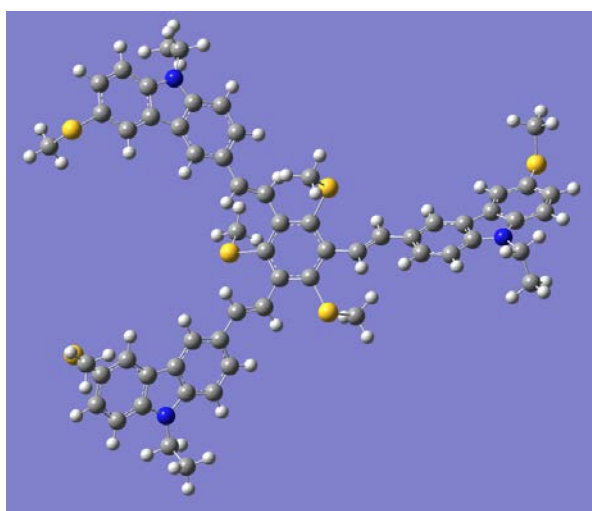
M3



M4



M5



M6

Fig.2 Optimized structure of the studied compounds obtained by B3LYP/6-31G (d, p) level.

Ci-Cj	TECEB	(M1)	(M2)	(M3)	(M4)	(M5)	(M6)
C11-C7	1.467	1.474	1.478	1.462	1.478	1.269	1.481
C8-C8	1.349	1.345	1.344	1.352	1.347	1.351	1.346
C8-C22	1.465	1.464	1.665	1.460	1.466	1.465	1.466
C17-C22	1.457	1.476	1.477	1.460	1.478	1.468	1.474
C18-C17	1.349	1.344	1.345	1.353	1.346	1.351	1.346
C18-C60	1.464	1.464	1.465	1.459	1.466	1.465	1.465
C12-C16	1.467	1.477	1.474	1.461	1.477	1.476	1.473
C12-C13	1.349	1.344	1.345	1.352	1.347	1.315	1.347
C13-C41	1.65	1.464	1.465	1.459	1.465	1.385	1.466
Θ_1	-178.3	173.69	172.72	-176.17	-167.42	-172.93	176.52
Θ'_1	0.448	-10.063	176.35	-156.40	-167.48	171.67	-128.31
Θ''_1	1.096	173.69	-175.82	151.94	-171.07	92.72	175.56
Θ_2	2.451	48.17	128.27	151.41	-135.05	-156.57	132.01
Θ'_2	-179	120.27	130.10	174.91	136.34	157.97	171.76

Θ''2	1.1	129.07	133.87	-179.54	-13.44	-173.95	136.38
------	-----	--------	--------	---------	--------	---------	--------

Table1: Geometric parameters (bond length (in Å) and inter-ring twisting angle (°) of optimized compounds M1, M2, M3, M4, M5 and M6 obtained by B3LYP/6-31G(d,p) in their neutral state.

The optimized inter-ring bond lengths and dihedral angles between the subunits are summarized in table1. We note firstly that the dihedral angle Θ_1' increases from M1 to M2 in this order M1<M6<M3<M4<M5<M2. The dihedral angle Θ_1'' increase from M5 to M2 in this order M5<M3<M4<M1<M6<M2. The dihedral angle Θ_2 increase from M1 to M5 in this order M1<M2<M6<M4<M3<M5 and

the dihedral angle Θ_2' increase from M1 to M3 in this order M1<M2<M4<M5<M5<M3. Secondly we note that the incorporation of several groups does not change the inter-ring distances (C7-C8) (C8-C22) (C17-C22) (C18-C17) (C18-C60) (C12-C16) and (C12-C13), but a slight increase in the distance (C11-C7) and (C13-C41) is observed for M5.

Table2: The theoretical electronic properties (HOMO, LUMO and Egap) (in eV) of the studied compounds calculated from the optimized structures by B3LYP/6-31G (d, p).

Compounds	HOMO(eV)	LUMO(eV)	Egap(eV)
M1	-5.202	-1.379	3.823
M2	-5.244	-1.361	3.882
M3	-5.760	-2.679	3.081
M4	-5.409	-1.676	3.732
M5	-4.617	-0.995	3.622
M6	-4.911	-1.293	3.618
TECEB	-4.860	-1.109	3.752

The values of HOMO and LUMO energies of M1 to M6 are (-5.202,-1.379), (-5.244,-1.361), (-5.760,-2.679), (-5.409,-1.676), (-4.617,-0.995), (-4.911,-1.293), (-4.860,-1.109 for TECEB) eV respectively. It can moreover be found that the HOMO and LUMO energies of the studied compounds are a little 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 TECEB ring on the HOMO and LUMO energies is clearly seen. The energies of Egap of the studied molecules change slightly from 3.882eV to 3.081eV depending on the different structures. They are classified in the following order:

$$M2 > M1 > M4 > M5 > M6 > M3.$$

3.2 Photovoltaic property

In general the HOMO and the LUMO energy levels of the donor and acceptor compounds are very important factors to determine whether effective

charge transfer will happen between donor and acceptor. We know that LUMO energy levels the ITO conduction band edge (-4.7 eV) is much lower than that the six studied compounds. These

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

We use the equation (1) for calculated of Voc, so we obtained the values of this open circuit voltage .The

molecules in excited states of M1, M2, M3, M4, M5 and M6 have a strong ability to inject electrons into ITO electrodes. Figure 4 shows detailed data of absolute energy of the frontier orbital for studying compounds and acceptor. The new acceptors they are the 56π-electron fullerene derivatives with LUMO levels C60(Ind)(CN₂) (1) (-3.87eV), C60(Qm)(CN₂) (2) (-3.88eV), C60(CH₃)(CN₃) (3) (-3.96eV), C60(QM)(CN₂)(Me) (4) (-3.75eV), C60(Ind) (-3.76eV), C60(Qm) (-3.78eV), C60(CH₂) (-3.8eV), PCBM (-3.8eV), DCMB (-3.8eV), C60(-3.89eV), SIMEFC (-3.74eV) were synthesized by Y-Abe et al.[12]. It should be noted that the LUMO levels of the studied compounds Mi (i=1-6) are higher than that of 56π-electron fullerene derivative. We have compared the HOMO and LUMO levels to investigate the possibilities of the electron transfer from the donor molecules (Mi) to the conductive band of the acceptor compounds (56π-electron fullerene derivative). The maximum open circuit voltage (Voc) of the BHJ solar cell is related to the difference between HOMO of the donor and the LUMO of the electron acceptor (56π-electron fullerene derivatives). We don't forget the energy gone during the photo-charge generation [13]. As a result the Voc (open-circuit voltage) follows by expression:

Voc of the studied compounds range from 0.357 eV to 1.72 eV (see Table 3) 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 compound to the conduction band of acceptor (56 π -electron fullerene derivative) and the

consequent is possible in an organic sensitized solar cell.

Table 3: Energy values of E_{LUMO} (eV), E_{HOMO} (eV) and the open circuit voltage V_{oc} (eV).

Cpds	HOMO	LUMO	E _{gap}	V _{OC}	α	V _{OC}	α	V _{OC}	α	V _{OC}	α
M1	-5.202	-1.379	3.823	1.032	2.491	1.022	2.501	0.942	2.581	1.152	2.371
M2	-5.244	-1.361	3.882	1.074	2.509	1.064	2.519	0.984	2.599	1.194	2.389
M3	-5.76	-2.679	3.081	1.59	1.191	1.58	1.201	1.5	1.281	1.71	1.071
M4	-5.409	-1.676	3.732	1.239	2.194	1.229	2.204	1.149	2.284	1.359	2.074
M5	-4.617	-0.995	3.622	0.447	2.875	0.437	2.885	0.357	2.965	0.567	2.755
M6	-4.911	-1.293	3.618	0.741	2.577	0.731	2.587	0.651	2.667	0.861	2.457
1		-3.87									
2		-3.88									
3		-3.96									
4		-3.75									
C60 (Qm)		-3.78									
C60 (Ind)		-3.76									
C60 (CH2)		-3.8									
PCBMe		-3.8									
DCBM		-3.8									
SIMEFC		-3.74									

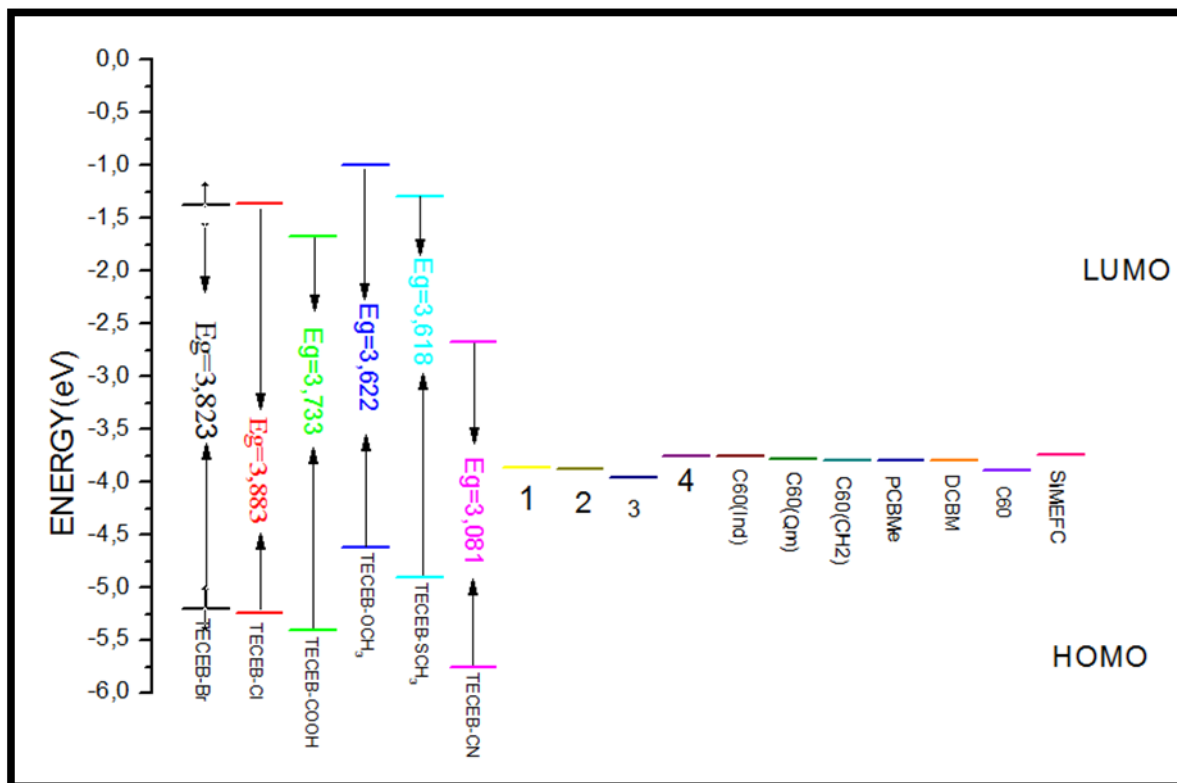
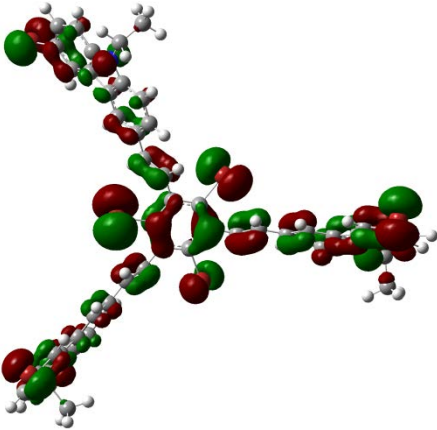
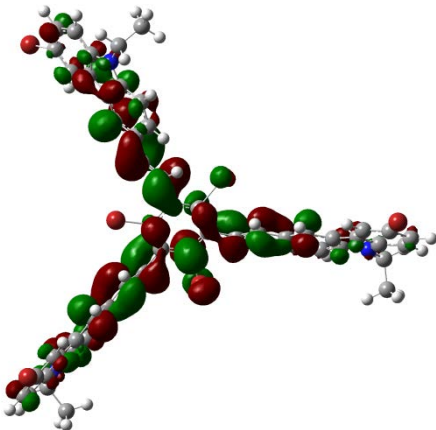
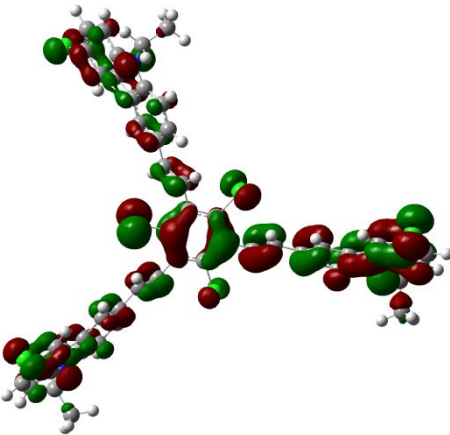
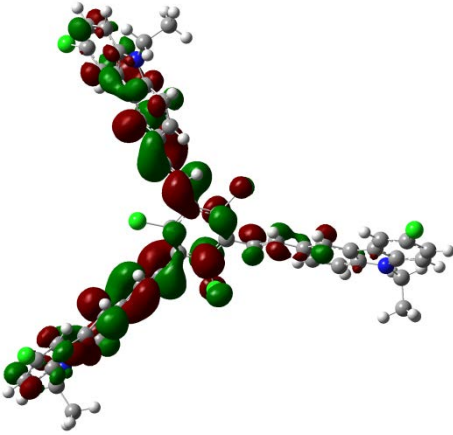
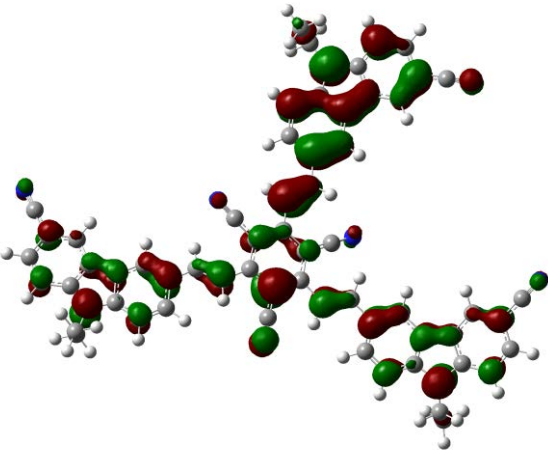
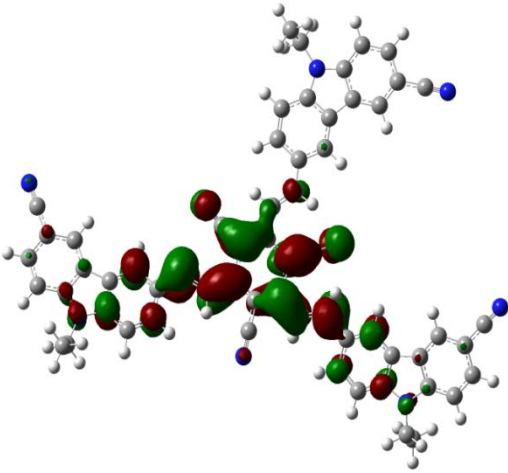


Fig. 4 Sketch of DFT/B3LYP/6-31G (d,p) calculated energy of the HOMO. LUMO levels of studied molecules.

3.3 Opto-electronic properties

The frontier molecular orbital (MO) contribution is very important in determining the charge-separated states of the considered compounds since the relative ordering of occupied and virtual orbital gives a reasonable qualitative indication of excitations properties [14]. As exposed in figure 5, the HOMOs

of these compounds in the neutral form possess a π -bonding character within subunit and a π -anti bonding character between the consecutive subunits; on the other hand the LUMOs possess a π -anti bonding character within subunit a π -bonding character between the subunits.

	HOMO	LUMO
M1		
M2		
M3		

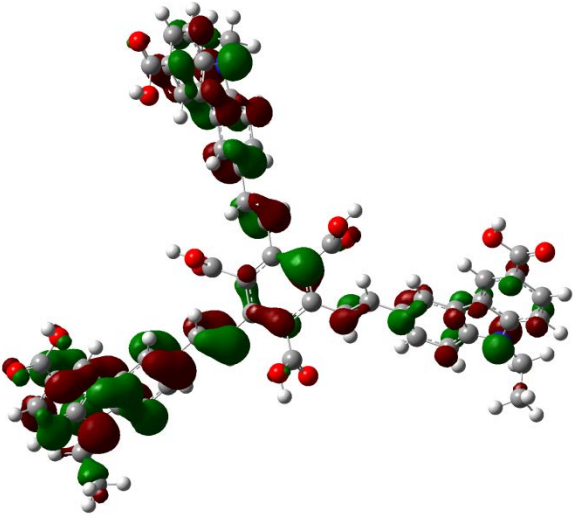
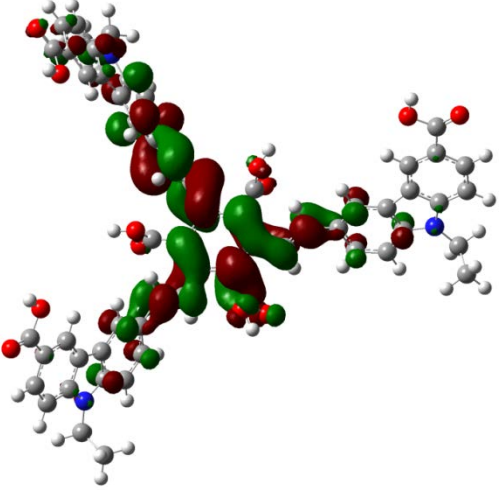
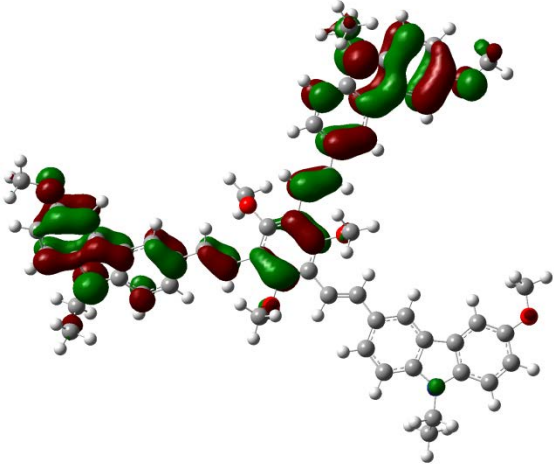
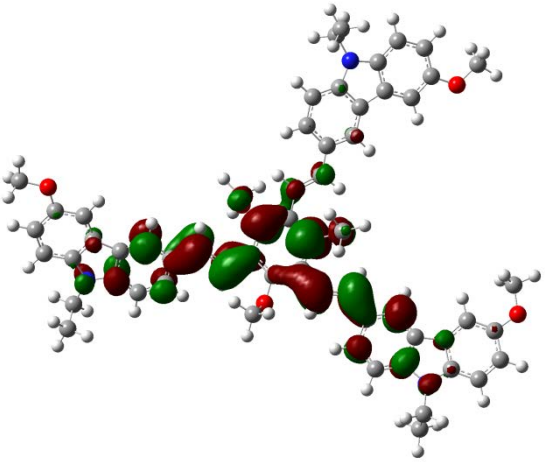
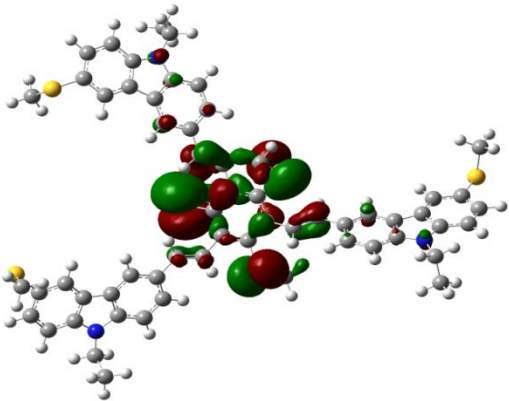
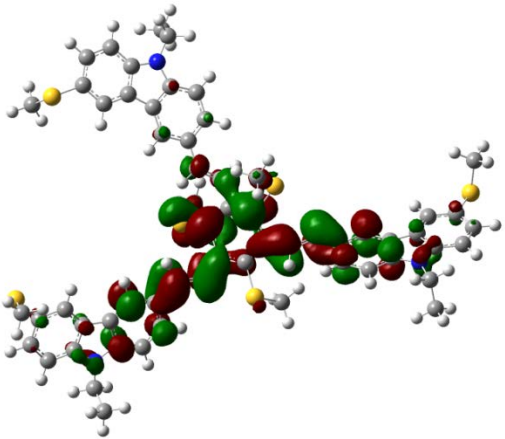
M4		
M5		
M6		

Fig. 5 Obtained isodensity plots of the frontier orbital HOMO and LUMO of the studied compounds obtained at B3LYP/6-31(d, p) level

3.4 Absorption and properties

Generally, how the absorption of a new material match with the solar spectrum is an important factor for the application as a photovoltaic material, and a good photovoltaic material should have broad and strong visible absorption characteristics. In fact we have calculated the UV-Visible spectra of the

studied compounds M_i ($i=1$ to 6) using TD-DFT starting with optimized geometry obtained at B3LYP/6-31G (d, p) level.

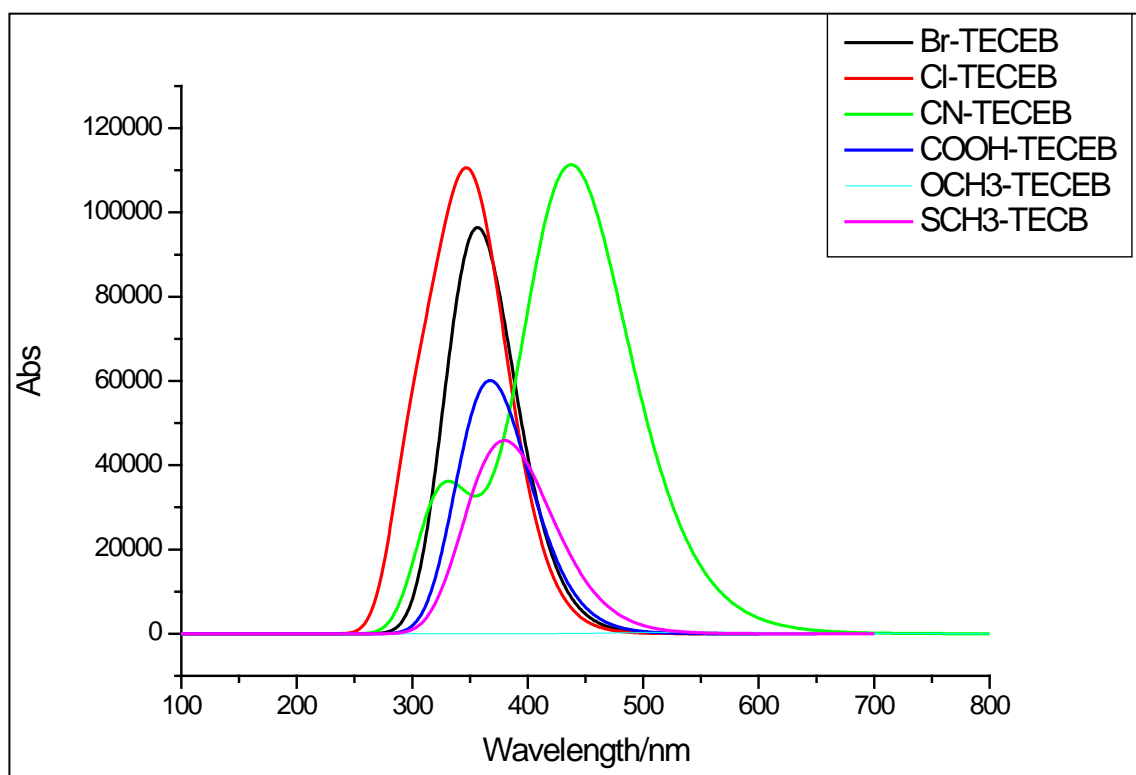


Fig6. Simulated UV-visible optical absorption spectra of each compound with the calculated data at the TD-DFT B3LYP/6-31G (d, p) level.

As illustrated in table 5, we can find the values of calculated wavelength λ_{max} and oscillator strengths O.S and compositions in terms of molecular orbital contributions. The promotion of an electron from the

HOMO to the LUMO results in excitation from S_0 to S_1 state. The absorption wavelengths arising from $S_0 \rightarrow S_1$ electronic transition increase progressively with the increasing of conjugation length.

Table 3: Main transition states, their assignments, the corresponding wavelength and oscillator strength for the title compounds by TD-DFT//B3LYP/6-31G (d, p).

Compounds	Wavelength (λ .nm)	E (ev)	O.S	Mo/Character
M1	371.5413	3.3369	0.3176	HOMO->LUMO (11%). HOMO->L+1 (76%)

				H-1->LUMO (7%)
	360.4271	3.4398	0.6512	H-1->L+1 (14%). HOMO->LUMO (70%). HOMO->L+1 (11%)
	357.5789	3.4672	0.6865	H-1->LUMO (74%)
	349.12098	3.5512	0.663	H-2->LUMO (42%). H-2->L+1 (13%). H-1->L+1 (27%)
	342.202358	3.6230	0.0163	H-2->LUMO (25%). H-1->L+1 (35%)
	340.66971	3.6393	0.0289	H-2->LUMO (13%). H-2->L+1 (70%)
	337.8568	3.6696	0.0742	H-2->L+2 (14%). H-1->L+4 (13%). HOMO->L+2 (32%). HOMO->L+4 (14%)
	337.41553	3.6744	0.015	H-1->L+3 (17%). HOMO->L+4 (30%)
	336.3993	3.6855	0.0247	H-1->L+1 (10%). H-1->L+3 (22%). HOMO->L+3 (26%)
	364.6246	3.4002	0.2353	H-1->LUMO (13%). HOMO->L+1 (82%)
	354.3292	3.49903	0.9891	H-1->L+1 (25%). HOMO->LUMO (62%)
	353.9145	3.50313	0.7699	H-1->LUMO (71%). HOMO->L+1 (12%) H-2->L+1 (7%)
	344.6374	3.5974	0.3789	H-2->LUMO (55%) .H-1->L+1 (13%). HOMO->LUMO (24%)
	339.3085	3.653931	0.0054	H-2->LUMO (15%). H-2->L+2 (12%). H-1->L+1 (32%). HOMO->L+2 (16%)
	337.9029	3.669130	0.0307	H-2->L+1 (72%)
	336.0346	3.68953	0.083	H-2->L+2 (10%) .H-2->L+3 (10%). H-1->L+3 (12%). HOMO->L+2 (29%)
	335.5072	3.69533	0.0388	H-2->L+1 (12%). H-1->L+3 (17%). H-1->L+4 (14%). HOMO->L+4 (32%) H-3->L+1 (3%). H-2->L+4 (9%)
	333.9258	3.712830	0.0203	H-2->LUMO (10%). H-2->L+2 (10%). H-1->L+1 (26%). HOMO->L+3 (13%)
	313.5088	3.954625	0.2711	HOMO->L+3 (29%). HOMO->L+5 (43%)
	310.6806	3.990624	0.1504	H-1->L+2 (25%). H-1->L+3 (12%). H-1->L+5 (16%).
M2				

				HOMO->L+4 (22%)
	309.3705	4.00752447	0.0454	H-1->L+2 (32%). H-1->L+3 (14%). HOMO->L+3 (24%)
	307.6127	4.03042	0.0552	H-1->L+2 (14%). H-1->L+4 (33%). HOMO->L+4(17%). HOMO->L+5 (27%) HOMO->L+3 (6%)
	306.7527	4.041723	0.0774	H-2->L+2 (24%). H-1->L+5 (35%). HOMO->L+2 (21%)
	305.475	4.05862	0.0595	H-2->L+2 (23%). H-1->L+2 (21%). H-1->L+5 (27%). HOMO->L+2 (13%)
	301.7360	4.108922	0.0057	H-4->L+1 (10%). H-3->LUMO (11%). H-2->L+3 (21%). H-2->L+5 (19%)
	299.650	4.137522	0.0277	H-3->L+1 (17%). H-2->L+3 (28%). H-2->L+4 (12%). H-1->L+3 (13%)
	298.9279	4.147521	0.1874	H-4->LUMO (10%). H-3->L+1 (30%). H-2->L+3 (17%)
	298.3237	4.155921	0.1945	H-5->LUMO (18%). H-4->L+1 (18%). H-2->L+4 (31%)
	298.008	4.160321	0.1661	H-4->L+1 (18%). H-2->L+4 (34%) H-5->LUMO (9%).
M3	473.8880	2.616250	0.1436	H-1->L+1 (10%). HOMO->LUMO (85%)
	444.7194	2.787847	0.5213	H-2->LUMO (67%). H-1->LUMO (29%) HOMO->L+1 (2%)
	441.1433	2.810447	1.0179	H-2->LUMO (24%). H-1->LUMO (36%). HOMO->L+1 (29%)
	432.8875	2.864046	0.8765	H-1->L+1 (77%). HOMO->LUMO (11%)
	422.1859	2.936644	0.1358	H-2->L+1 (95%)
	410.6632	3.019043	0.1086	H-1->LUMO (26%). HOMO->L+1 (66%)
	373.612	3.31843746	0.0375	H-4->LUMO (18%). H-3->LUMO (73%)
	371.9648	3.333137	0.0049	H-4->LUMO (71%). H-3->LUMO (18%)
	370.37591	3.34743691	0.0475	H-5->LUMO (92%)
	363.9503	3.406535	0.0322	H-3->L+1 (81%)
	355.1310	3.491134	0.0121	H-4->L+1 (84%)
347.8086	3.564632	0.0023	H-5->L+1 (94%)	

	331.010	3.745529	0.228	H-6->LUMO (39%). HOMO->L+2 (35%)
	329.0864	3.767429	0.3089	H-7->LUMO (10%). H-6->LUMO (13%). H-2->L+3 (16%). H-1->L+2 (18%).
	326.6243	3.7958	0.0116	H-7->LUMO (12%). HOMO->L+2 (13%). HOMO->L+5 (10%)
	326.2633	3.800028	0.0913	H-7->L+1 (14%). H-6->LUMO (18%). H-1->L+2 (21%). H-1->L+4 (12%)
	322.059	3.849627	0.0089	HOMO->L+2(21%). HOMO->L+5 (38%)
	320.5608	3.867627	0.1792	H-2->L+3 (13%). H-1->L+2 (45%).
	316.8336	3.913125	0.0049	H-7->LUMO (41%). H-2->L+2 (36%)
	312.1119	3.972325	0.0071	H-7->LUMO (27%). H-2->L+2 (35%)
M4	380.3869	3.259338	0.353	HOMO->LUMO (92%)
	365.0863	3.395936	0.8843	H-2->LUMO (27%). H-1->LUMO (54%) . HOMO->L+1 (15%)
	360.8047	3.436235	0.2845	H-2->LUMO (63%). H-1->LUMO (29%) H-1->L+1 (4%)
M5	564.7414	2.195358	0.0	H-1(A)->LUMO(A) (24%). HOMO(B)->L+1(B) (24%)
	552.3873	2.244457	0.005	HOMO(A)->LUMO(A)(12%). HOMO(A)->L+1(A) (22%). HOMO(A)->L+2(A) (47%).
	538.6130	2.301856	0.0045	HOMO(A)->LUMO(A) (18%). HOMO(A)->L+1(A) (14%). HOMO(A)->L+2(A) (41%). H-2(B)->LUMO(B) (2%)
M6	398.8013	3.108841	0.4493	HOMO->LUMO (89%)
	383.7067	3.231139	0.3041	HOMO->L+1 (83%)
	362.3019	3.422035	0.5188	H-1>LUMO(66%). H-1->L+1 (21%)

We based the optimization of the studied compounds M_i ($i = 1-6$) for calculation the UV-Vis spectra by using TD/DFT at B3LYP/6-31(d, p) level. As illustrated in Table 3, we found the values of calculated wavelength λ_{max} and O.S. The promotion of an electron from the HOMO to the LUMO result in excitation from S_0 to S_1 state. These values were calculated by TD/DFT method starting with the optimized geometry obtained at B3LYP/6-31G(d,p) level. M1 shows a series of bands between 336.399 and 371.5413 nm, and the strongest absorption at 357.5789 nm belonging to

the HOMO to LUMO transition. M2 depicts a series of bands between 298.008 and 364.624 nm, and the absorption at 354.3292 nm could be assigned to the electronic transition from HOMO to LUMO. M3 puts forward a series of bands between 312.112 and 473.888 nm, and the absorption at 441.1433 nm is attributed to the electronic transition from HOMO-1 to LUMO. M4 depicts a series of bands between 360.8047 and 380.3869 nm, and the absorption at 365.0863 nm could be assigned to the electronic transition from HOMO-1 to LUMO. M5 depicts a series of bands between 538.6130 and 564.7414 nm,

and the absorption at 538.6130 nm could be assigned to the electronic transition from HOMO(A) to LUMO+2. M6 depicts a series of bands between 362.3019 and 398.8013 nm, and the absorption at 398.8013 nm could be assigned to the electronic transition from HOMO to LUMO. Data in Table 3 show that there is a bathochromic shift when passing from M2 to M5 in the following order M2→M1→M4→M6→M3→M5 which also can be seen respectively in M2 (354.3292 nm), M1 (357.5789 nm), M4 (365.0863 nm), M6 (398.8013 nm), M3 (441.1433 nm) and M5 (538.6130 nm). This effect is obviously due to insertion of different donor or acceptor into the p-spacer units. This seems evident when we study the electronic and absorption properties.

4. Conclusions

In this study, the quantum chemical investigation on the geometries and electronic properties of various new compound carbazole derivatives is performed in order to display the effect of molecular structure on the opto-electronic properties of these materials and to see 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 have similar confirmations (quasi flat conformation). We discover that the introduction of several groups does not change the bond length (C7-C8), (C8-C22), (C176-C22), (C18-C17), (C18-C60), (C12-C16) and (C12-C13) but a slight increase in the distance (C11-C7) and (C13-C41) is observed for M5.

➤ We calculated the energy gaps (LUMO-HOMO) we found that the energy gaps of the studied molecules differ slightly from **3,882 eV to 3,081 eV** depending on the different structures. So we can classify these compounds in the following order:

$$M2 > M1 > M4 > M5 > M6 > M3.$$

- Comparing the values obtained after substitution indicate that CN substitution reduces the LUMO, HOMO and Egap from **3,75 eV to 3,081 eV** and increases the absorption maximum, λ_{max} , from **351,46 nm to 441,1433 nm**.
- The energy Egap of molecule 6CN-TECEB (M3) is much smaller than that of the other compounds.
- All the studied molecules can be used as sensitizers, because the electron injection process from the excited molecule to the conduction band of 56π -electron fullerene derivatives and the

subsequent regeneration are feasible in the organic sensitized solar cell.

- The best values of Voc are indicated for the studied compounds blended with SMIFEC and the higher value is given for molecule M3 blended with SMIFEC (**1,72 eV**).

Acknowledgements

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

References

- [1] H. S. Nalwa, Ed. John Wiley & Sons (October 1999), E. Lim, B.-J. Jung, H.-K. Shim, T. Taguchi, B. Noda, T. Kambayashi, T. Mori, K. Ishikawa, H. Takezoe, L.-M. Do, Handbook of Organic Conductive Molecules and Polymers, Org. Electron. 7, 121, 2006
- [2] C. D. Dimitrakopoulos and P. R. L. Malenfant, "Organic Thin Film Transistors for Large Area Electronics", Adv. Mater, Vol. 14, 2002, pp. 99-117,
- [3] A. KRAFT, A. C. GRIMSDALE, and A. B. HOLMES, "Electroluminescent conjugated polymers: seeing polymers in a new light", Angew. Chem Int Ed Engl, Vol. 37, 1998, pp. 402-428.
- [4] A. G. Manoj, K. S. Narayan, "Photovoltaic properties of polymer p-n junctions made with P3OT/BBL bilayers", Opt. Mater, Vol. 21, 2003, pp. 417.
- [5] K. Müllen, G. Wegner (Eds.), Electronic Materials : The oligomers Approach, Wiley-VCH, Weinheim, New York, 1998, pp. 105-197, J. Cornil, D. Beljonne, J. L. Brédas, K. Müllen, G. Wegner (Eds.) Electronic Materials : The oligomers Approach, Wiley-VCH, Weinheim, New York, 1998, pp. 432-447 (and the references therein)
- [6] M. Velusamy, K. R. J. Thomas, J. T. Lin *et al.* "Organic dyes incorporating low-band-gap chromophores for dye-sensitized solar cells". Organic Letters, Vol. 7, No 10, 2005, pp. 1899-1902.
- [7] LI, Jiuyan, LIU, Di, LI, Yanqing, et al. "A high Tg carbazole-based hole-transporting material for organic light-emitting devices". Chemistry of materials, vol. 17, No 5, 2005, pp. 1208-1212.

- [8] C Lee, W Yang, R G Parr. *Physical Review B*, Vol. 37, 1988, pp 785-789.
- [9] (a) A. D. Becke, *Chem. Phys.*, Vol. 98, 1993, pp. 5648-5652. (b) S. H. Vosko, L. Wilk, M. Nusair, *Canadian J. Phys.*, Vol. 58, 1980, pp 1200-1211.
- [10] 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. JDannenber, 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. *GAUSSIAN03. Revision B.4*, Gaussian. Inc. Pittsburgh PA, 2003.
- [11] S. Bouzakraoui, S. M. Bouzzine, M. Bouachrine, M. Hamidi, *J. Sol. Energ. Mater. & Sol. Cells*, Vol. 90, 2005, pp. 1393.
- [12] Y. Abe, T. Yokoyama, Y. Matsuo, *Organic Electronic*, Vol.14, 2013, pp 3306-3311.
- [13] He-ping Shi, Jian-xin Dai, Li-wen Shi, Lei Xu, Zhao-bin Zhou, Yan Zhang. Wen Zhou, Chuan Dong, *Spectrochimica Acta Part*, Vol 93, 2012, pp. 19– 25.
- [14] M. C. Scharber, D. Mühlbacher, M. Koppe, P. Denk, C. Waldauf, A. J. Heeger, C. J. Brabec, “Design Rules for Donors in Bulk-Heterojunction Solar Cells—Towards 10 % Energy-Conversion Efficiency”, *J. Adv. Mater.* Vol.18, 2006, pp. 789–794.