

Chapter

Synthesis, Experimental and Theoretical Investigations on the Optical and Electronic Properties of New Organic Active Layer for a New Generation of Organic Light-Emitting Diode

Mourad Chemek, Ali Mabrouk, Mourad Ben Braieck, Jany Wéry Ventirini and Alimi Kamel

Abstract

In this chapter, we present new attempts for the development of a new generation of high-performance organic light-emitting diodes (OLEDs). First of all, we present two strategies for obtaining a luminescent active layer. The first one is the chemical synthesis of a block copolymer based on the cross-linked Poly (N-vinyl carbazole) (PVK) and the conjugated poly(3-methylthiophene) (PMeT) system. Secondly, newly small luminescent organic molecules are chemically synthesized and studied. Photo-physical and electronic properties of the synthesized organic materials are fully investigated through experimental analysis and theoretical computations using essentially DFT and TDDFT methodologies. Optical measurements revealed the formation of a new highly luminescent organic material. Furthermore, the newly synthesized small molecules showed a high emission in the blue part. Based on the synthesized active layers, newly multi-structure OLED architectures are theoretically designed by the insertion of a single-walled carbon nanotube (SWCNTs) as a single layer. The theoretical computations show that the insertion of single-walled carbon nanotubes (SWCNTs) single layer improves the injection of electron charge carriers from the chosen cathode (Ca, Mg) to the synthesized active layers, which enhances the performance of the electronic focused devices based on the organic synthesized active layer.

Keywords: organic light-emitting diode (OLEDs), poly(N-vinyl carbazole) (PVK), single-walled carbon nanotube (SWCNTs), DFT methodologies, small molecules

1. Introduction

The progress of the research in the field of Organic electronic devices based on organic materials has been actually a considerable challenge for scientific chemistry and physics [1–3]. The use of conjugated polymers such as Poly(p-phenylene vinylene) (PPV) derivatives was permitted to obtain flexible and transparent green OLEDs [4, 5]. Else, the extension of the effective conjugated length in poly(3-alkyl thiophene) (PAT) family, enhances the π - π stacking effects in the condensed state [6, 7], consequently, a poor red emission in the condensed state, is obtained with a weak photoluminescence quantum efficiency (PLQY), which is at around 1–2%, limiting also the use of PAT conjugated polymers for OLED applications [6, 7]. In order to enhance the photophysical properties of the investigated organic active layer of the organic light-emitting diode (OLEDs) and to improve the performance of the OLEDs displays, many efforts have recently been undertaken on the photoactive layer [8, 9]. Furthermore, experimental and theoretical efforts on the multilayer structure were employed in order to enhance the performance of the focused displays [8–10]. Recently, focused researchers show that Carbazole or bicarbazole based conjugated polymers are among superior host materials, showing promising performances in newly organic light-emitting devices [11–14]. Moreover, the use of small molecules is one of the new solutions to minimize the geometric distortion and the possible defect on the main chain and to enhance the investigated photophysical properties [8–10]. In this area of research, we have firstly, incorporated Poly(9-vinyl carbazole) (PVK) under the chemical polymerization of 3-methyl thiophene monomers, using the anhydrous Ferric chloride (FeCl_3) in chloroform solution [15]. The new polythiophene derivative is named PVK-MeT [15]. Photophysical investigations based essentially on spectroscopic analysis show a great enhancement in the luminescence properties, which encourage the investigation of the new material for a new generation of OLED devices [15, 16]. On the other hand, we present the chemical synthesis of a new blue-emitted organic small molecule [17]. Two newly synthesized organic materials are obtained and named respectively 1,4-Bis(a-cyano-4-methoxystyryl) benzene (DOMCN) and 1,4-Bis(a-cyano-4-bromostyryl)benzene (DBrCN) [17]. The chemical synthesis of the DOMCN and DBrCN molecules is done for possible investigation as an active layer for a new generation of a new performant organic blue light-emitting diode. The chemical synthesis and the photophysical properties were briefly described herein, and theoretical computations are undertaken to determine the electronic parameters of the synthesized chemical structure. Moreover, the synthesized organic materials presented in this chapter were theoretically used as an active layer in a newly designed multilayer structure for organic light-emitting display using essentially Density functional theory (DFT) computations on the geometric and electronic structure of the optimized chemical structure. Theoretical investigations show that The insertion of single-walled carbon nanotubes (SWNTs) on the prepared multilayer structure enhances the injection of the charge carriers (electron) and improves the physical and electronic performance of the electronic devices based on the investigated organic materials.

2. Experimental and computational details

Optical absorption measurements were carried out at room temperature (RT) using a Varian Cary 5G spectrophotometer. Photoluminescence excitation (PLE)

measurements were recorded with Continuous-wave photoluminescence measurements (PL), which were collected on a Jobin-Yvon Fluorolog 3 spectrometer using a Xenon lamp (450 W). Quantum chemical computations were performed using density functional theory (DFT) and TDDFT methodologies of calculation [18], and using B3LYP functional coupling with the 6-31G (d) basis set [19, 20]. DFT and TDDFT methodologies of calculations are frequently used for a better description of the structural, photophysical and electronic properties of organic synthesized materials [21, 22]. The geometry of the first excited state was obtained by the re-optimization of the ground state optimized geometry with the configuration interaction singles restricted (RCIS) ab initio method (RCIS/6-31G(d)) [23]. Used methodologies of calculation are implemented in Gaussian 09 program [24].

3. Chemical synthesis and experimental properties of the news organics active layers

3.1 Brief description of the chemical synthesis and Photophysical properties of the PVK-MeT

The chemical synthesis of the PVK-MeT starts with the cross-linking of the Poly(9-vinylcarbazole) (PVK) in presence of 3-(methyl thiophene) monomers in chloroform solution using the anhydrous ferric chloride (FeCl_3) as an oxidant. The material was obtained in the doped state and the neutral state was fully obtained by chemical treatment described elsewhere in our previous paper [15]. The neutral and doped states were identified essentially by analyzing the obtained samples by infrared and Raman analysis as well as optical absorption tools to prove the successful de-doping of the sample [15].

3.2 Photo-physical properties of the PVK-MeT

Optical absorption spectra of the synthesized material PVK-MeT was first investigated by optical absorption and PLE spectroscopies in chloroform diluted solution. Obtained spectra are presented in **Figure 1**. The synthesized material absorbs essentially in the UV-visible part, with an intense narrow absorption centered at around 250 nm and a shoulder absorption band centered at 410 nm. The PLE spectrum registered for the investigated material in the solution state of 550 nm maximum emission, shows a maximum at around 410 nm, coinciding with the maximum absorption assigned to π - π^* optical transition. As mentioned above, poly (3-alkyl thiophene) and in particular Poly(3-methyl thiophene) synthesized by FeCl_3 routes absorbs essentially in the visible part with an intense absorption located at around 500 nm in the condensed state [25].

In order to study the excited state of the synthesized organic material, the sample was excited under various excited lines going from UV to visible part using first steady-state photoluminescence spectroscopy. No optical signal is obtained under UV excitation and a high emission is obtained under visible excitation, confirming PLE results. On the second step, PVK-MeT and PMeT powder were then excited under 400 nm laser pulsed excitation and the PL obtained spectra are presented in **Figure 2**.

From **Figure 2**, it is clearly seen that the PL intensity is improved upon using the Poly(N_vinylcarbazole) (PVK) on the chemical synthesis of the Poly (3-methyl thiophene) (PMeT) by FeCl_3 oxidative polymerization routes. In contrast with the PL

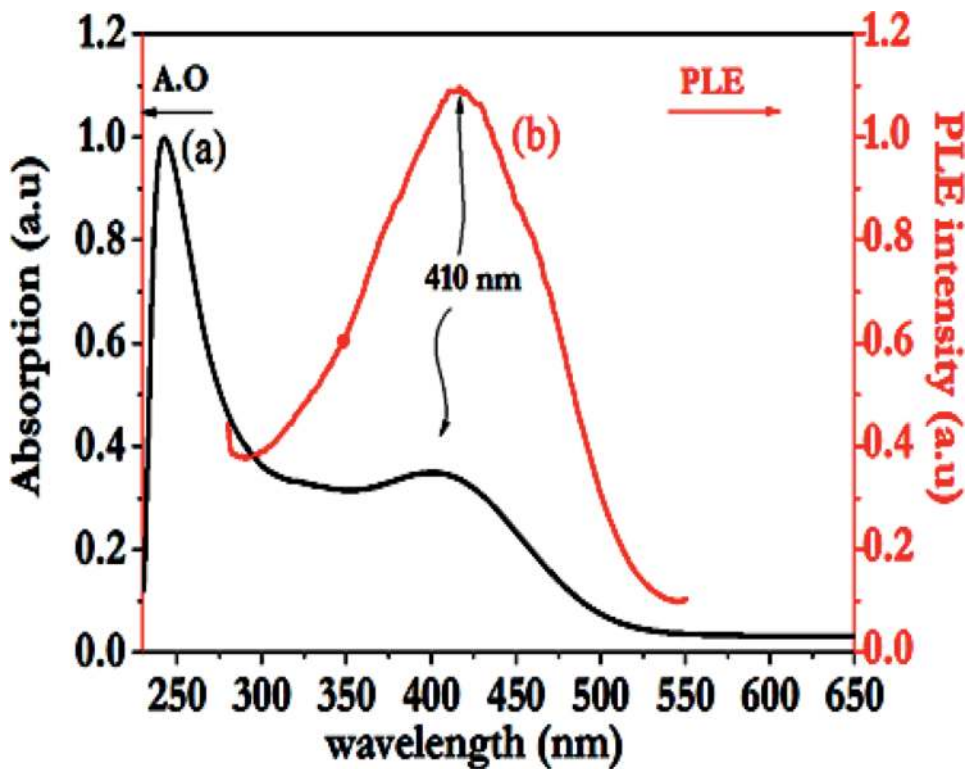


Figure 1. Optical absorption (a) and PLE spectra (b) of the synthesized PVK-MeT.

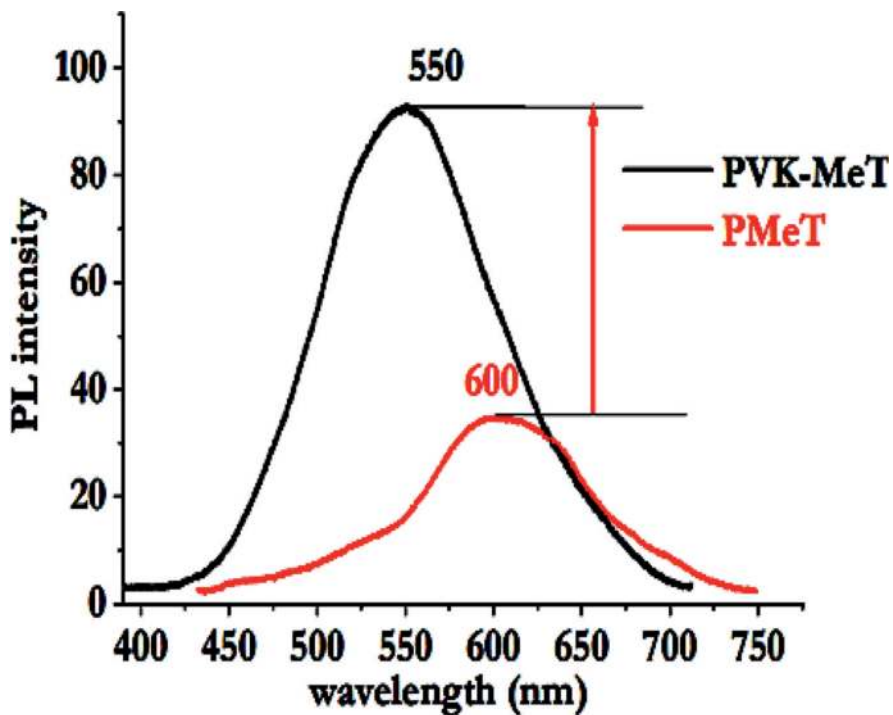


Figure 2. Photoluminescence spectra of PVK-MeT and PMeT powder (excitation 400 nm).

spectrum of PMeT, PVK-MeT exhibits an intense emission (see **Figure 2**). Indeed, we calculate the ratio I_1/I_2 , where, I_1 and I_2 present respectively the maximum intensity of the PL spectra of the PVK-MeT and that of the PMeT homopolymer. The ratio is at around 4. An emissive active layer based on thiophene derivative was successfully obtained. The improvement of the luminescence properties is accompanied by a blue shift of the maximum emission from 600 nm to 550 nm, showing a change in the spectral emission, which is shown by the CIE cartographic (See **Figure 6**). The enhancement of the luminescence properties is confirmed by the analysis of the PL decays analysis using transient photoluminescence analysis on the synthesized PVK-MeT and PMeT homopolymer powder, described in detail in our previous paper [23]. Transient photoluminescence spectroscopy confirms the change of the nature of the photogenerated species going from PMeT to PVK-MeT, which induce an increase of the PLQY from 1 to 2% for poly(3-alkylthiophene) [6, 16] to 13% for PVK-MeT in the condensed state [16].

Theoretical computations based essentially on DFT-B3LYP-6-31G(d) level of theory, was permitting to deduces first the chemical structure of the synthesized material and their electronic parameters such as HOMO, LUMO energies, and the energy gap

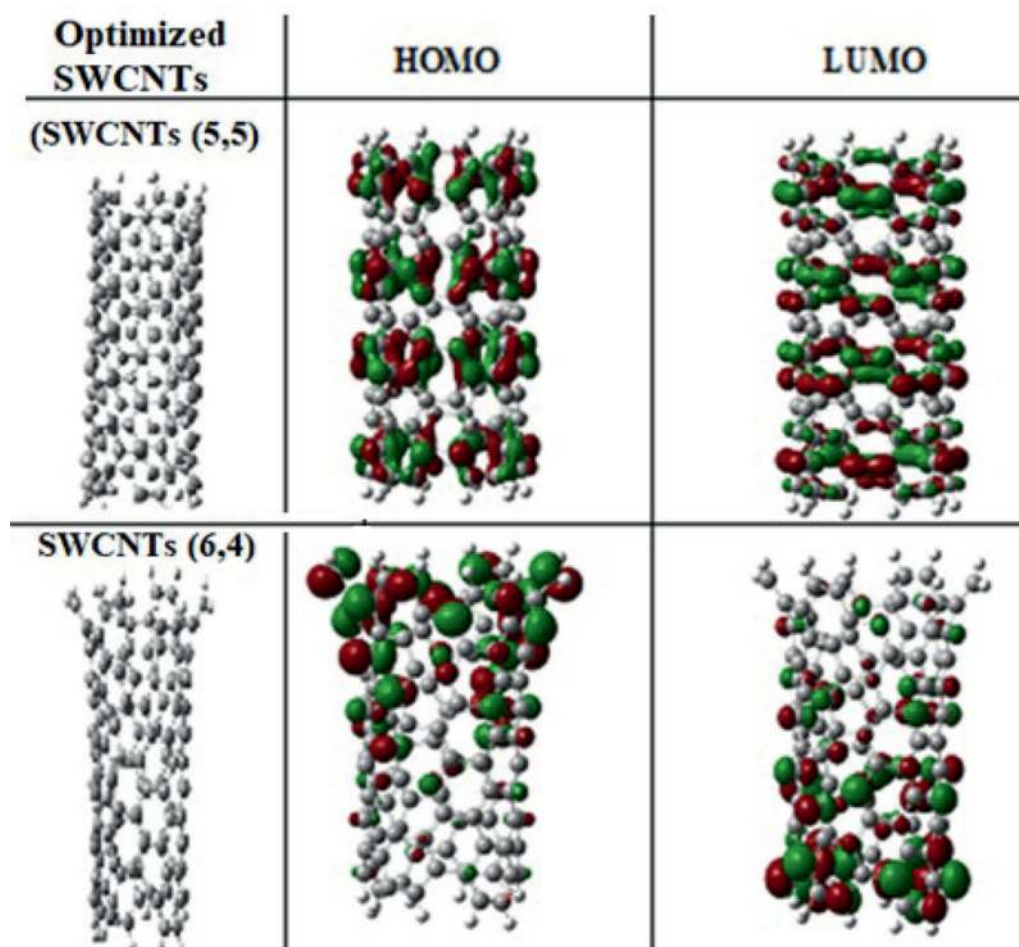


Figure 3. Optimized chemical structure of (SWCNTs) (5,5) and (SWCNTs) (6,4) and their contour plot HOMO and LUMO.

Photoactive layer	EHOMO (eV)	ELUMO (eV)	Eg (eV)	IP (eV)	EA (eV)
DOMCN	-5.41	-2.27	3.14	5.41	2.27
DBrCN	-5.98	-2.80	3.18	5.98	2.8
Pv PVK-MeT	-4.8	-1.8	3	4.8	1.8

Table 1.
Electronic parameters of the investigated organic active layer.

HOMO-LUMO. The ionization potential (I.P) and electron affinity (E.A) are theoretically deduced using Koopman's theorem [26]. Obtained results are summarized in **Table 1**. Polythiophene derivatives and in particular Poly(3-methylthiophene) (PMeT) present a good absorption in the visible part and a red light emission is produced, when the PMeT homopolymer is excited by the visible line [27]. Else, in a condensed state (thin film) a low emission is produced with a low photoluminescence quantum yield (PLQY), which is at around 1–2% [6, 28]. The planarity of the chemical structure on the excited state of pol(3-alkylthiophenes) derivative, favors the formation of the non-emissive excimer species under the photo-excitation (excited state) [6, 28]. Further, the high π -conjugated system in polythiophenes favors the formation of the π - π stacking on the condensed state, which enhances the fast migration mechanism of the photo-generation species [6, 28, 29]. Consequently, non-radiative pathways are favored and a poor emission signal is obtained with fast multi-exponential decays are produced [29, 30].

In order to study the structure-properties relationship of the investigated materials, first, a simple optimization on the ground state of an oligomer of 6-thiophenes coupled at the 2–5 positions and of the deduced chemical structure of the PVK-MeT. Secondly, the fully optimized chemical structures on the first excited state are

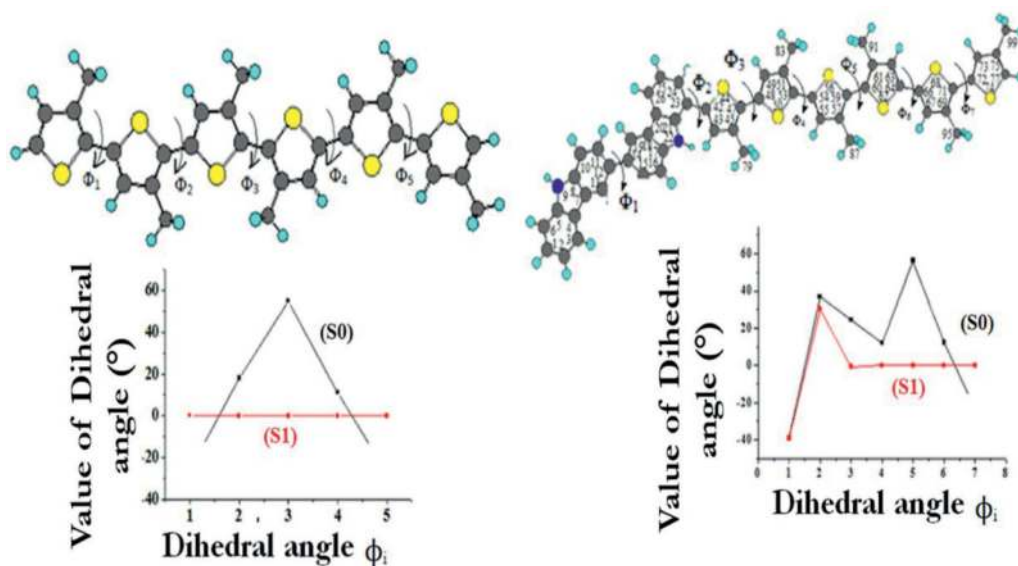


Figure 4.
Geometric parameters (dihedral angle ϕ_i) of the optimized chemical structure of the six-coupled non-regioregular 3-(methyl thiophene) and the PVK-MeT chemical structure on the ground (black line) (S0) and the first calculated excited state (S1) (red line).

successfully obtained by re-optimization of the optimized ground-state chemical structure with the RSCI/6-31G(d) level of theory. The optimized chemical structures on the ground and the first excited state are drawn with Gauss view software and presented in **Figure 4**.

Geometric parameters such as dihedral angle ϕ of 6-Oligothiophene optimized in the ground and the first excited-state state are presented in **Figure 4**. It is clearly seen from **Figure 4**, that the conformation of the non-regioregular coupled 3-methyl thiophene presents a non-planar conformation, and the distortion is higher on the TT coupling (ϕ_3) in the ground state. Else, the first excited state of the non-regioregular 6-oligothiophene, obtained by the re-optimization of the optimized chemical structure by CIS/STO-3G present no distortion and a fully coplanar structure. Focused studies reveal that the luminescence in the conjugated system is only obtained when the main chain is deformed especially in the excited state [26]. Indeed, Bai et al. [6], suggest that upon excitation of the conjugated system in poly (3-alkyl thiophene), the planarity increases, which favors the formation of the nonemissive excimer species in the condensed state [6]. Consequently, a poor luminescence with low PLQY is obtained for polythiophenes derivatives in the condensed state [6]. Herein, the insertion of the cross-linked carbazole system (bicarbazole) grafted to the 6-oligothiophene system induces the increase of the distortion and the high deformation of the main chain in both grounds and excited state (**Figure 3**). These behaviors induced the decrease of the non-radiative photo-generated species and the improvement of the luminescence properties going from PMeT to PVK-MeT.

3.3 Chemical elaboration of new small molecules for OLEDs application

3.3.1 Chemical synthesis of news small molecule: DOMCN and DBrCN

To an equimolar stirred mixture of 1,4- phenylenediacetonitrile (1) (1 mmol) and aldehyde (2) (2 mmol) in 10 mL of tert-butyl alcohol (10 mL) were added a solution of tetrabutylammonium hydroxide (TBAH) (1 M solution in methanol). After 24 h of stirring at 50°C, the reaction mixture was cooled to room temperature and quenched with distilled water. Then, the obtained solution was extracted with chloroform. The organic layer was washed several times with distilled water and dried over anhydrous magnesium sulfate. The purification was carried out by precipitation in methanol. A yellow powder was filtered and dried in a vacuum for 24 h (**Figure 5**).

¹H NMR (CDCl₃) δ [ppm]: 7.89 (d, 4H, Ar-H), 7.71 (s, 4H, Ar-H), 7.49 (s, 2H, Vinyl-H), 6.96 (d, 4H, Ar-H), 4.04 (t, 6H, -OCH₃). ¹³C NMR (CDCl₃) δ [ppm]: 160.5, 142.4, 135.1, 131.5, 126.2, 126.2, 118.5, 115.1, 107.5, 68.1.

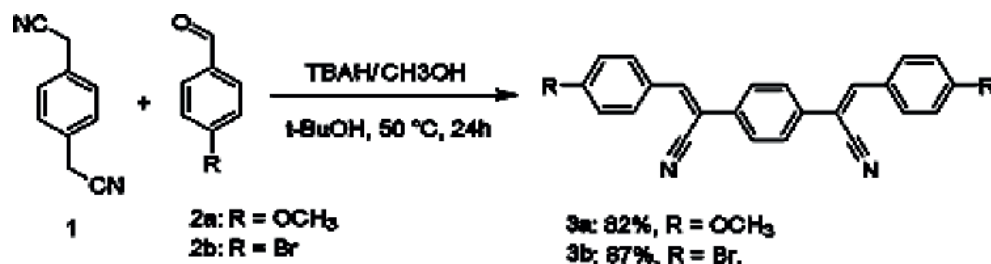


Figure 5.
The synthesis adopted procedure of the DOMCN and DBrCN.

3.3.2 Photo-physical properties of the synthesized DBrCN and DOMCN

Optical properties of the synthesized oligomer were investigated essentially with steady-state optical absorption and photoluminescence spectroscopies in a dilute solution state. Optical absorption and photoluminescence spectra are presented in **Figure 6**. Both synthesized molecules absorb in the UV and in the near-visible part. A wide absorption is detected at 250 nm and a large band absorption centered at around 360 nm and 380 nm respectively for DBrCN and DOMCN synthesized molecules, and are assigned to π - π^* optical transition. From optical absorption spectra, optical band gap E_g is estimated from the onset of absorption, which is estimated to be 3 eV and 2.8 eV respectively for DBrCN and DOMCN molecules.

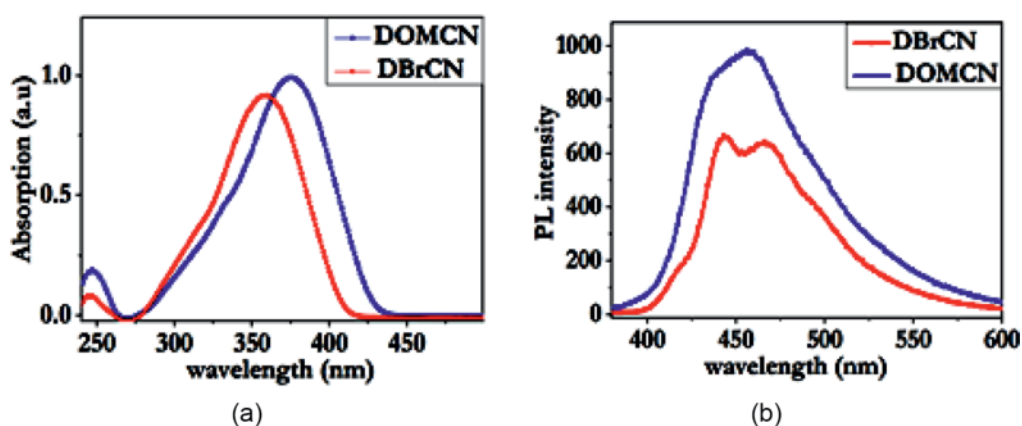


Figure 6. (a) Optical absorption and (b) photoluminescence spectra (excitation 370 nm) of the DOMCN and DBrCN synthesized molecules recorded in chloroform solution.

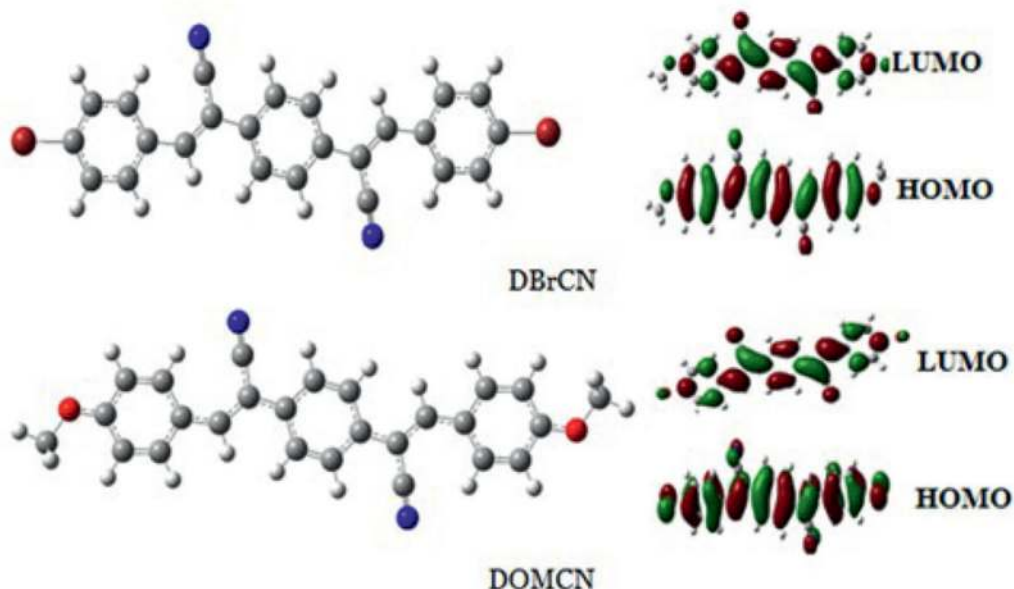


Figure 7. Optimized chemical structure and their contour plots orbitals HOMO and LUMO of DOMCN and DBrCN.

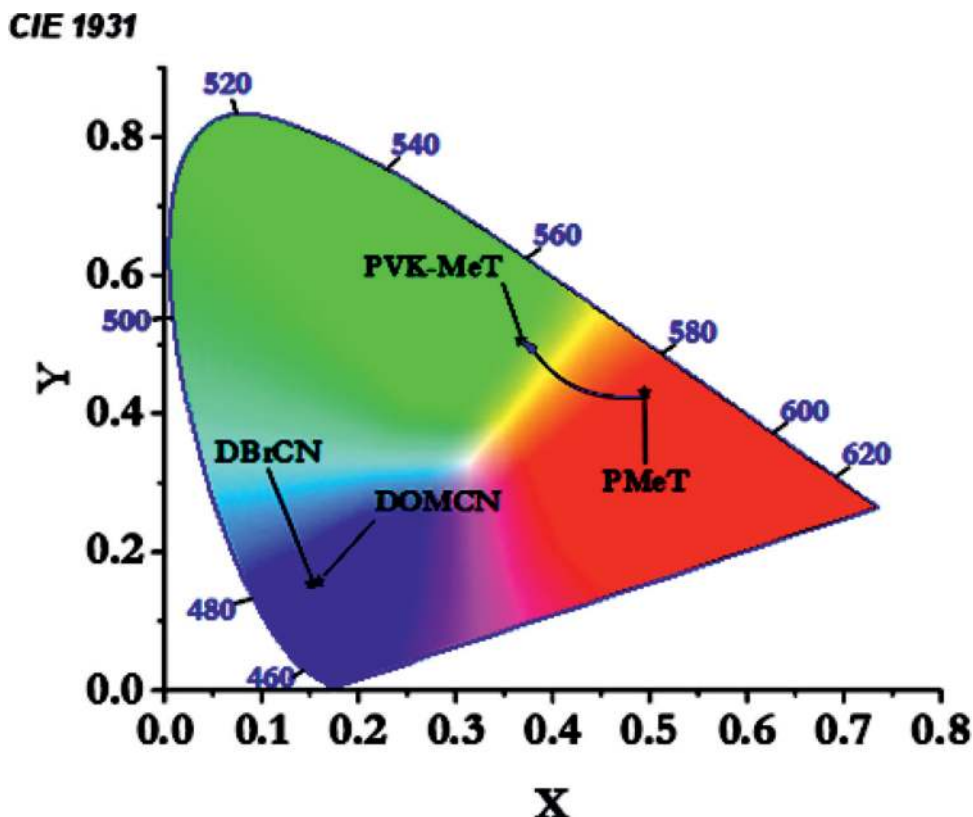


Figure 8.
C.I.E cartographic of the investigated organic material.

Under 370 nm line excitation a narrow blue emission is observed for the two materials. A change in the shape of the PL spectrum of the molecule is observed going from DBrCN and DOMCN. A vibronic spectrum with two maxima at 443 and 460 nm for DBrCN is obtained. Theoretical computations using the DFT-B3LYP-6-31G(d) level of theory were undertaken in order to estimate the electronic parameter. **Figure 7** presents the optimized chemical structure of the investigated molecule at the ground state and the contour plot HOMO and LUMO obtained with 0.02 isovalue using GAUSSVIEW software [27].

Electronic parameters deduced from the ground state optimized chemical structure of the two compounds and the synthesized PVK-MeT are summarized in **Table 1**.

From CIE cartography (**Figure 8**), it is clearly seen the effect of the use of Poly(N_vinylcarbazole) (PVK) on the chemical polymerization of 3-methylthiophene monomers. From PMeT to PVK-MeT a decrease of x value from 0.5 for single PMeT to 0.38 for PVK-MeT resulted in a green-yellow color emission. Meanwhile, the synthesized small molecule DOMCN and DBrCN present a blue emission, which permits the use as an emissive layer for the blue light-emitting diode.

4. Theoretical design of new multilayer architecture based on the synthesized materials

Recently, Organic light-emitting diodes (OLEDs) have been considerably developed and considerable progress in the efficiency and durability is obtained [28, 29]. In order

to improve the injection and transport of the charge carriers from the anode or cathode, special multi-layer architectures are needed [30]. In this way, we are going in this part to the theoretical design of a new multilayer architecture using the investigated materials as an active layer. The first step of the calculations consists of the optimization of the geometries of the two single-walled carbon nanotube (SWCNTs) (5,5) and (6,4) having a diameter $\phi = 0.71$ nm and length $L = 100$ nm (150 atoms), with the DFT-B3LYP-6-31G(d) level of theory. The two optimized chemical structures are presented in **Figure 3**.

From the optimized chemical structure of the two forms of single-walled carbon nanotubes, the electronic parameters such as E_{HOMO} , E_{LUMO} , and the energy gap $E_g = E_{HOMO} - E_{LUMO}$ were deduced and summarized in **Table 2**.

4.1 Energy diagram of an OLED based on these compounds

In this part, we attempt to design new organic architecture using the luminescent investigated material as an active layer by the insertion of single-walled carbon nanotubes as shown in **Figure 9**.

First, the anode and cathode must be chosen to facilitate the injection of the free charge carrier from anode or cathode to the active layer (luminescent organic material). **Table 3** presents the traditionally used material and their electronic characteristics parameters (anode output work (Φ_A) and the output work of the cathode (Φ_C)).

By comparing electronic parameters of the investigated material and that of The traditional anode and cathode materials, cathode (Ca, Mg) can better helpfully inject the charge carriers (electron) from the cathode to the synthesized materials. Using

	E_{HOMO} (eV)	E_{LUMO} (eV)	I.P (eV)	E.A (eV)	$E_g = E_{HOMO} - E_{LUMO}$ (eV)
SWCNTs (5,5)	-4.30	-2.93	4.3	2.93	1.37
SWCNTs (6,4)	-3.94	-3.54	4.3	3.54	0.40

Table 2.

Electronic parameters of the optimized chemical structure of SWCNTs (5,5) and SWCNTs (6,4).

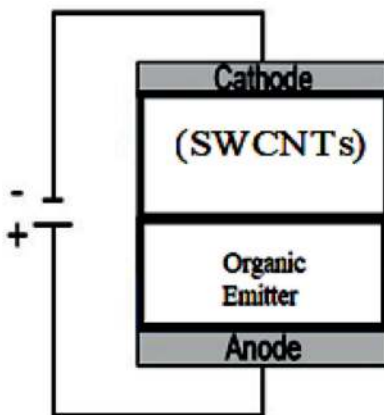


Figure 9.

Proposed multilayer structure using the investigated organic material as an emitting layer.

Anode	Cathode
ITO; $\Phi_A = 4.7$ eV	Ca, Mg; $\Phi_C = 2.90$ eV
ITO:PEDOT-PSS, $\Phi_A = 5.20$ eV	Al, Ag; $\Phi_C = 4.30$ eV
	Au; $\Phi_C = 5.00$ eV

Table 3.
 Value of the work function of the possible used cathode and anode.

Anode	Cathode	Active layer	ΔE_e (eV)	Active layer- SWCNTs	ΔE_e (eV)	
ITO $\Phi_A = 4.7$ eV	ITO: PEDOT-PSS $\Phi_A = 5.20$ eV	(Ca, Mg) $\Phi_C = 2.90$ eV	PVK-MeT	1.1	PVK-MeT/ SWCNTs (5,5)	0.03
					PVK-MeT/ SWCNTs (6,4)	0.64
			DMOCN	0.63	DOMCN / SWCNTs (5,5)	0.03
					DOMCN/ SWCNTs (6,4)	0.64
				0.1	DBrCN/ SWCNTs (5,5)	0.03
					DBrCN/ SWCNTs (6,4)	0.64

Table 4.
 Electronic parameters of the possible used anode and cathode and the active layer with and without SWCNTs.

(Ca, Mg) as a chosen cathode in the designed multi-structure layer, and the synthesized materials (PVK-MeT, DMOCN and DBrCN) as an active layer, we calculate the electron injection barrier (ΔE_e), which is defined as the energy difference between the energy value of the LUMO of the used photoactive layer and the output work of the cathode (Φ_C). The obtained results are summarized in **Table 4**. The insertion of the single-walled carbon nanotube (SWCNTs) between the cathode and the photoactive layer

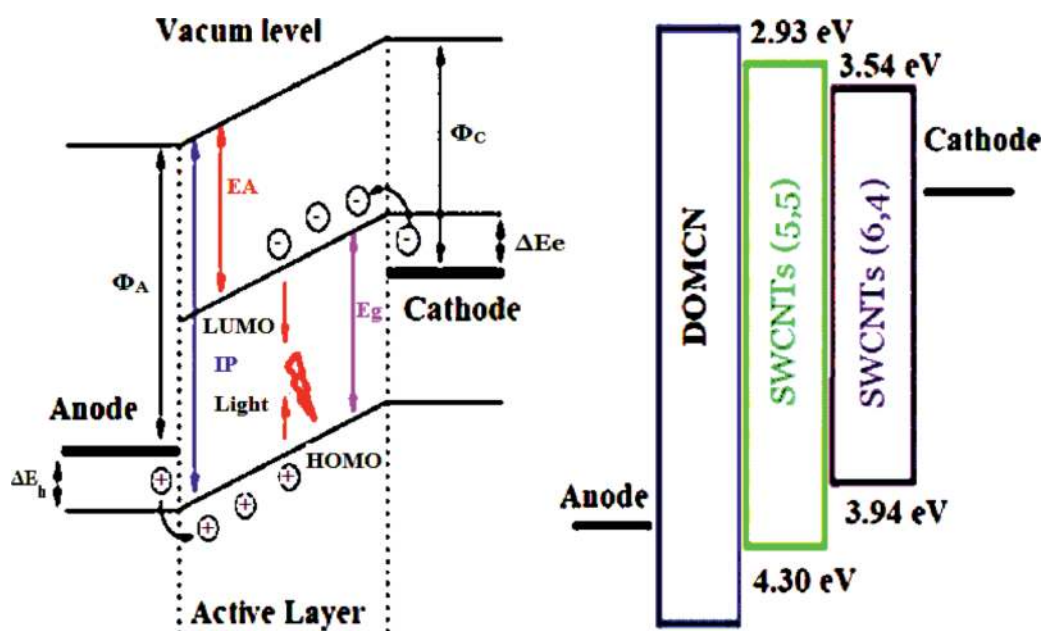


Figure 10.
 Energetic diagram of the designed OLEDs based on the investigated organic material.

greatly reduces the value of ΔE_e . The reduction of ΔE_e is more important with SWCNTs (5,5) than when using the SWCNTs (6,4) reduction (see **Figure 10**).

Consequently, SWCNTs (5,5) as a layer between the (Ca, Mg) and the investigated photoactive multilayer can helpfully improve the electron injection from the cathode to the active material which improves the performance of The OLEDs based on the designed multi-structure.

5. Conclusions

In summary, we have attempted in the present chapter to enhance the optical emission and electronic properties of the chosen organic emitting layer for a new generation of the organic light-emitting diode (OLED). The first step is to use the non-conjugated Poly(Vinylcarbazole) (PVK) in the chemical synthesis of the conjugated polymers (case Poly(3-methyl thiophene)). The use of PVK under the chemical synthesis of the poor luminescent Poly(3-alkylthiophene) family permits first the partially crosslinking of the carbazole units, which enhances the PL intensity and improves their luminescence properties. Elsewhere, the use of a new family of small molecules permits also to obtain a blue luminescent organic material with reduced non-radiative recombination of hole and electron. The chemical structures of the synthesized materials were used as an active layer in newly simulated light-emitting devices. DFT simulations on the investigated materials and in the simulated devices show that the introduction of the optimized layer of single-walled carbon nanotubes (SWCNTs) single layer permits to the enhancement of the electron injection and improves the performance of the focused emitting devices.

Acknowledgements

This study was funded by the Ministry of Higher Education and Scientific Research-Tunisia: Synthèse asymétrique et ingénierie moléculaire de matériaux organiques pour l'électronique organique (LR18ES19). Authors are grateful to Dr. Florian Massuyeau and to Eric Faulques for their help on the optical measurements done at IMN Nantes (France).

Author details


Mourad Chemek^{1*}, Ali Mabrouk¹, Mourad Ben Braieck¹, Jany Wéry Ventirini²
and Alimi Kamel¹

1 Faculté des Sciences de Monastir, Synthèse asymétrique et ingénierie moléculaire de matériaux organiques pour l'électronique organique (LR18ES19), Monastir, Tunisie

2 Institut des Matériaux Jean Rouxel, Nantes cedex 3, France

*Address all correspondence to: chmek_mourad@yahoo.fr

IntechOpen

© 2022 The Author(s). Licensee IntechOpen. This chapter is distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/3.0>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited. 

References

- [1] AlSalhi MS, Alam J, Dass LA, Raja M. Recent advances in conjugated polymers for light emitting devices. *International Journal of Molecular Sciences*. 2011; **12**(3):2036-2054. DOI: 10.3390/ijms12032036
- [2] Grimsdale AC, Leok Chan K, Martin RE, Jokisz PG, Holmes AB. Synthesis of light-emitting conjugated polymers for applications in electroluminescent devices. *Chemical Reviews*. 2009; **109**(3):897-1091. DOI: 10.1021/cr000013v
- [3] Zhang C, Braun D, Heeger AJ. Light-emitting diodes from partially conjugated poly(*p*-phenylene vinylene). *Journal of Applied Physics*. 1993; **73**(10):5177. DOI: 10.1063/1.353794
- [4] Burn PL, Homes AB, Kraft A, Bradley DDC, Brown AR, Friend RH. Synthesis of a segmented conjugated polymer chain giving a blue-shifted electroluminescence and improved efficiency. *Journal of Chemical Society, Chemical Communications*. 1991:32-34. DOI: 10.1039/C39920000032
- [5] Grem G, Leditzky G, Ullrich B, Leising G. Realization of a blue-light-emitting device using poly(*p*-phenylene). *Advanced Materials*. 1992; **4**:36. DOI: 10.1002/adma.19920040107
- [6] Xu B, Holdcroft S. Molecular control of luminescence from poly(3-hexylthiophenes). *Macromolecules*. 1993; **26**:4457-4460. DOI: 10.1021/ma00069a009
- [7] Ng SC, Xu JM, Chan HSO. Electrically conductive and fluorescent poly[1,4-bis(3-alkyl-2-thienyl)phenylenes]: Syntheses and preliminary characterization aspects. *Synthetic Metals*. 1998; **92**:33-37. DOI: 10.1016/S0379-6779(98)80019-2
- [8] Chemek M, Chebil S, Ben Amor S, Khlaifa D, Faulques E, Haj Said A, et al. Chemical insertion of anthracene moiety into the backbone of a newly synthesized oligophenylene (OMPA): effect on the photo-physical properties. *Research on Chemical Intermediates*. 2021; **47**:3437-3451. DOI: 10.1007/s11164-021-04481-z
- [9] Bourass M, Kohima N, Keltoum Kabbaj O, Wazzan N, Chemek M, Bouachrine M. The photophysical properties and electronic structures of bis[1]benzothieno[6,7-*d*:6',7'-*d'*]benzo[1,2-*b*:4,5-*b'*]dithiophene (BBTBDT) derivatives as hole-transporting materials for organic light-emitting diodes (OLEDs). *New Journal of Chemistry*. 2019; **43**:15899-15909. DOI: 10.1039/C9NJ02756D
- [10] Wazzan N, Irfan A. Exploring the optoelectronic and charge transport properties of Pechmann dyes as efficient OLED materials. *Journal of Optik*. 2019; **197**:163200. DOI: 10.1016/j.ijleo.2019.163200
- [11] Bezikonny O, Grybauskaite-Kaminskiene G, Volyniuk D, Simokaitiene J, Danyliv Y, Durgaryan R, et al. 3, 3'-Bicarbazole-based compounds as bipolar hosts for green and red phosphorescent organic light-emitting devices. *Materials Science and Engineering: B*. 2020; **261**:114662. DOI: 10.1016/j.mseb.2020.114662
- [12] Liu X-Y, Zhang Y-L, Fei X, Liao L-S, Fan J. 9, 9'-Bicarbazole: New molecular skeleton for organic light-emitting diodes. *Chemistry A European Journal*. 2019; **25**/4501-25/4508. DOI: 10.1002/chem.201806314

- [13] Rui B, Tan Y, Liu X, Wei C, Liu Y, Li J, et al. Synthesis, characterization of bicarbazole compounds and their application in codepositing luminescent copper iodide complexes. *ChemistrySelect*. 2017;**2**:6556-6562. DOI: 10.1002/slct.201700742
- [14] Zhou R, Jin M, Malval J, Pan H, Wan D. Bicarbazole-based oxalates as photoinitiating systems for photopolymerization under UV-Vis LEDs. *Journal of Polymer Science*. 2020;**60**:1-13. DOI: 10.1002/pol.20199298
- [15] Chemek M, Wéry J, Bouachrine M, Paris M, Lefrant S, Alimi K. Synthesis and characterization of novel graft copolymers of Poly(N-vinylcarbazole) and Poly(3-methylthiophene) for optoelectronic applications. *Synthetic Metal*. 2010;**160**:2306-2314. DOI: 10.1016/j.synthmet.2010.09.001
- [16] Chemek M, Massuyeau F, Wéry J, Hlel A, Ayachi S, Faulques E, et al. Photoluminescence properties of new poly(N-vinylcarbazole)-3-methylthiophene (PVK-3MeT) graft copolymer. *Journal of Applied Polymer Science*. 2012;**125**:126-132. DOI: 10.1002/app.35074
- [17] Bouazizi H, Mabrouk A, Braïek MB, Mestiri T, Alimi K. New conjugated organic matrix-carbon nanotube functionalization: DFT modeling and spectroscopic analysis. *Journal of Physics and Chemistry of Solids*. 2020;**136**:109131. DOI: 10.1016/j.jpcs.2019.109131
- [18] Armelin E, Bertran O, Estrany F, Salvatella R, Alemán C. Characterization and properties of a polythiophene with a malonic acid dimethyl ester side group. *European Polymer Journal*. 2009;**45**:2211. DOI: 10.1016/j.eurpolymj.2009.04.010
- [19] Lee C, Yang W, Parr RG. *Journal of Physical Review B*. 1998;**37**:785
- [20] Becke AD. *The Journal of Chemical Physics*. 1996;**104**:1040
- [21] Hamroun I K, Hafedh N, Chmeck M, Aloui F. Photooxidation pathway providing 15-bromo-7-cyano [6] helicene. Chiroptical and photophysical properties and theoretical investigation. *Journal of Molecular Structure*. 2020;**1217**:128399. DOI: 10.1016/j.molstruc.2020.128399
- [22] Samaher C, Mourad C, Alimi K. Theoretical investigations about the effect of electron-withdrawing groups on properties of A- π -D- π -a type small molecules donor for organic solar cells. *Journal of Molecular Modeling*. 2021;**27**:54. DOI: 10.1007/s00894-020-04654-4
- [23] Belletête M, Bedard M, Leclerc M, Durocher G. *Journal of Molecular Structure (THEOCHEM)*. 2004;**9**:679
- [24] Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, et al. *Gaussian09 Revision D.01*. Wallingford: Gaussian Inc; 2009
- [25] Zhao L, Chen Q, Li C, Shi G. Electrochemical fabrication of p-poly(3-methylthiophene)/n-silicon solar cells. *Solar Energy Materials & Solar Cells*. 2007;**91**:1811-1815
- [26] Chemek M, Ayachi S, Hlel A, Wéry J, Lefrant S, Alimi K. A theoretical investigation on the properties of the new poly(N-vinylcarbazole)-3-methylthiophene (PVK-3MeT) synthesized graft copolymer. *Journal of Applied Polymer Science*. 2011;**122**:2391-2402
- [27] Wang L, Xian W, Wang X, Feng Q, Pei M, Zhang G. Synthesis and characterization of three novel conjugated polythiophene derivatives. *Designed Monomers and Polymers*. 2013;**16**:339-348. DOI: 10.1080/15685551.2012.747151

[28] Massuyeau F, Faulques E, Lefrant S, Majdoub M, Ghedira M, Alimi K, et al. Photoluminescence properties of new PPV derivatives. *Journal of Luminescence*. 2011;**131**: 1541-1544

[29] Massuyeau F, Duvail JL, Athalin H, Lorcy JM, Lefrant S, Wéry J, et al. Elaboration of conjugated polymer nanowires and nanotubes for tunable photoluminescence properties. *Nanotechnology*. 2009;**20**(15):155701. DOI: 10.1088/0957-4484/20/15/155701

[30] Monkman AP, Bloor D, Stevens GC. Electronic structure and charge transport mechanisms in polyaniline. *Synthetic Metals*. 1987;**21**:71. DOI: 10.1016/0379-6779(89)90307-X