

Theoretical Study on New Conjugated Compounds of Organic Solar Cell: DFT, TD-DFT and AMPS1D

EL Mhamedi I.^{1*}, El Karkri A.¹, EL Malki Z.¹, Bouachrine M.²

¹Modeling Materials and Systems Control (MMSC), Computer Engineering and Intelligent Electrical Systems (2ISEI) Laboratory, High School of Technology (ESTM), University Moulay Ismail, Meknes, Morocco,

²MCNS Laboratory, Faculty of Science, University Moulay Ismail, Meknes and EST Khenifra, Sultan Moulay Slimane University, Morocco,

*Corresponding author, Email address: i.elmhamedi@edu.umi.ac.ma

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Abstract: DFT and TD-DFT are used to examine a series of new conjugated compounds with small band gaps, intended for use in bulk heterojunction solar cells. The AMPS-1D program was used to simulate the performance of our compounds. These conjugated compounds carry the Triphenylamine donor unit, their conjugated bridge is based on Phenylenevinylene, and different π , 3, 4-Ethylenedioxythiophene (EDOT), carbazole, and thiophene systems. The 2-cyanoacrylic acid was used as the electron acceptor group. The calculated optimized geometries indicate that they all have coplanar structures. The HOMO (most occupied molecular orbital), LUMO (lowest unoccupied molecular orbital) levels, gap energy ($E_{\text{HOMO-LUMO}}$) and absorption spectrum wavelength (λ_{max}), as well as several quantum chemical properties such as open circuit voltage V_{oc} , ionization potential (IP), electron affinity (EA), have also been calculated and discussed in detail in the paper. The short circuit current density (J_{sc}), the form factor (FF) the power conversion efficiency (η), the series resistance R_{s} , and the shunt resistances R_{sh} are obtained using AMPS-1D. All these properties suggest that these compounds are good candidates for use in organic solar cells.

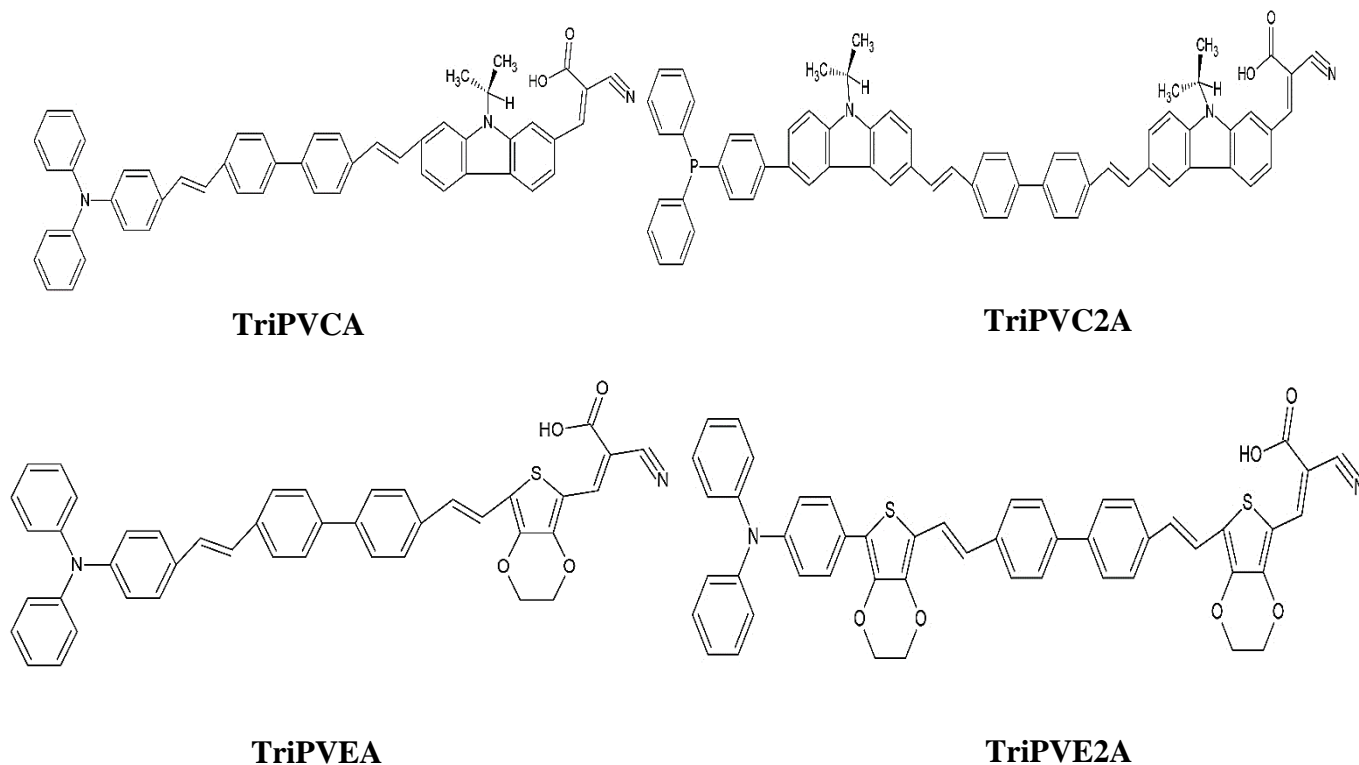
Keywords: Solar Cell; Donor-Acceptor; Thiophene; PCBM; Efficiency.

1. Introduction

The energy supplied by the sun in 1 hour is greater than the world's energy consumption for a whole year and the reference scenario of the International Energy Agency (IEA) predicts that the world's primary energy needs will increase by 55% between 2005 and 2030 ([world energy, 2007](#)). Nowadays, there is a considerable development of molecular materials based on π -conjugated systems; these systems were discovered in the 1970s on doping of polyacetylene, following the work of A. Hegger, Mc Diarmid and H. Shirakawa ([Al-Azzawi et al., 2023](#)). Various uses in the field of organic electronics are used as organic solar cells (OSCs), OLEDs, and field effect transistors ([Borshchev et al., 2021](#)). Since organic photovoltaics (OPVs) have attracted a lot of attention due to their various potential advantages, such as lightweight, easy to fabricate, flexible, and inexpensive devices ([Güney et al., 2019](#)). Since the donor- π -acceptor (D- π -A) components, which consist of an electron donor (D) and an electron acceptor (A) connected by a π -conjugated bridge (π -linker) possess molar absorption coefficients and their electronic properties can be easily tuned by molecular modifications. Many types

of D- π -A have been synthesized with enthusiasm (Bourass *et al.*, 2019). The role of the π -binding agent is not only to facilitate an intramolecular charge transport from the D-unit to the A-unit, but also to enhance the light-harvesting ability. Many researchers have developed electron donor materials with good solubility, low energy gap, optimized energy levels, broad absorption and high mobility (Duan *et al.*, 2012, Abram *et al.*, 2018). The interaction between electron donors (D) and electron acceptors (A) in a copolymer can result in the hybridization of the best occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, leading to a low energy gap organic semiconductor (Zahlou *et al.*, 2015). In order to increase the energy conversion efficiency of the photovoltaic device, by improving the charge transfer and exciton transport. Several conjugated compounds consisting of an alternating donor (D) and acceptor (A) with low band gap energy have been developed (Imelda *et al.*, 2022, EL Malki *et al.*, 2016, EL Malki *et al.*, 2018). Conjugated compounds are used as a donor in combination with fullerene derivatives ([6,6]-phenyl-C61-butyric acid methyl ester or PCBM) (Aicha *et al.*, 2019), which are widely used as acceptors in solution-processable photovoltaic devices, especially in combination with P3HT, due to its high electron mobility and remarkable electronic conductivity (Mhamedi *et al.*, 2022). Thiophene compounds were applied successfully in various fields such as pharmacology, agriculture and industrial applications as corrosion inhibitors of metals in aggressive media (Shah & Verma, 2018; Hawash *et al.*, 2022; Cetin *et al.*, 2019; Warad *et al.*, 2013; Bouklah *et al.*, 2004).

In this study, we examined a series of new organic compounds bearing the Triphenylamine donor unit, their conjugated bridge is based on Phenylenevinylene and various electron donor substituents: 3, 4-Ethylenedioxythiophene (EDOT), Carbazole, and Thiophene, and the electron acceptor group employed was 2-cyanoacrylic acid, this anchor group leads to a redder shift of the absorption bands. We focused on the theoretical study and quantum calculations of structural, electronic, optical properties by DFT/B3LYP/6-31G(d,p) density functional on Gaussian 09 software package, subsequently AMPS-1D program is used to study and simulate the photovoltaic properties. The geometrical structures are presented in **Figure 1**:



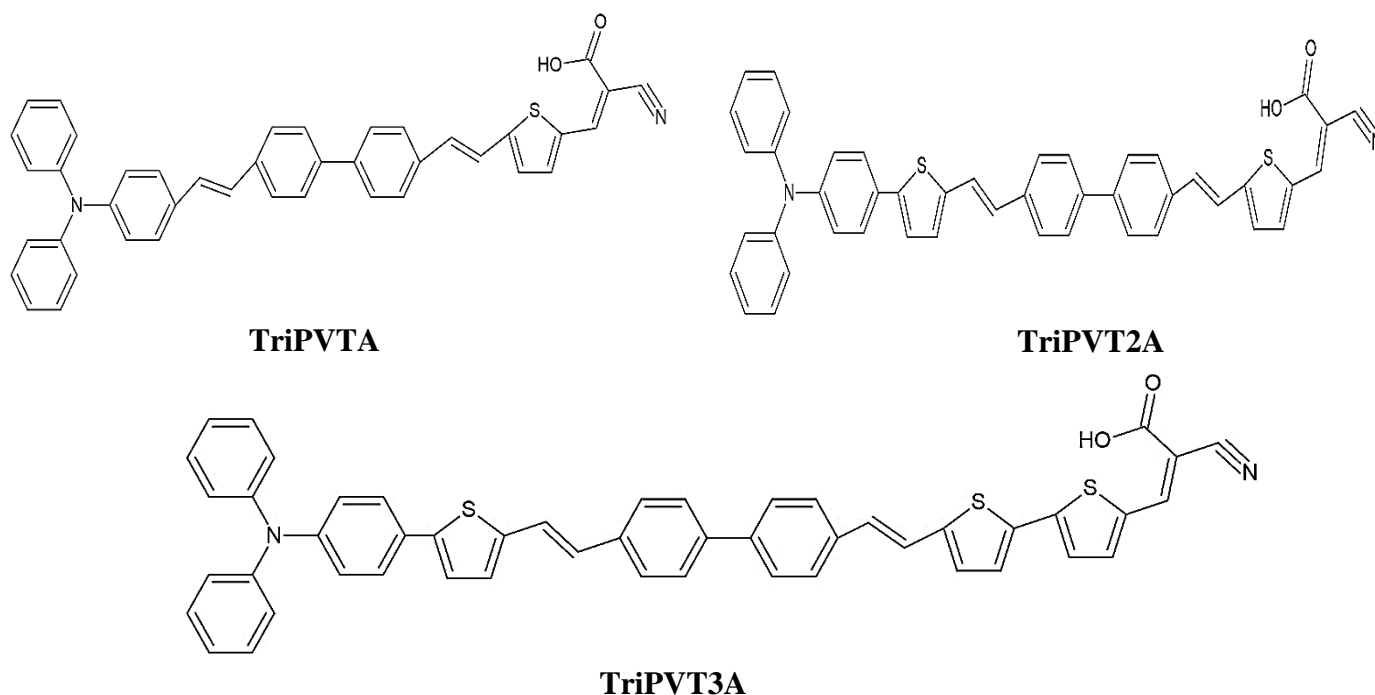


Figure 1. The sketch map structures of studied organic compounds

2. Computational method

2.1 DFT calculation

Molecular calculations were performed using density function theory (DFT) with the hybrid function B3LYP using the 6-31G (d,p) basis set of Gaussian 09 software, all optimizations were performed in the gas phase (Khlaifia *et al.*, 2020; Al Hamzi *et al.*, 2013). All optimizations were calculated without any symmetry constraints. The HOMO, LUMO and deviation (HOMO-LUMO) are also deduced for stable structures. The spatial distribution of (HOMO) and (LUMO) boundary orbitals provides a strategy by which the photovoltaic properties of solar cells can be understood. The vertical excitation energy, wavelengths, and electronic transition energies of the oligomers were obtained using time-dependent density function theory TD/DFT with B3LYP calculations.

2.2 AMPS1D

The Analysis of Microelectronic and Photonic Structures in One Dimension (AMPS-1D) program has been successfully used to study organic solar compounds. This simulation program solves the Poisson equation and the electron-hole continuity equations using the net difference method and the Newton-Raphson method and technique (Pennsylvania State University, 1997). The advantage of using simulation programs is the possibility to examine the influence of model parameters, which cannot be determined experimentally (El Karkri *et al.*, 2020).

3. Results and Discussion

3.1 Geometric and electronic structures

The dihedral angle and bond lengths between units in the polymer backbone have significant effects on the polymer conjugation, and thus, on the optoelectronic properties (Kacimi *et al.*, 2020). The geometry of these seven molecules was optimized by applying the DFT/B3LYP / 6-31G (d, p) method; all optimized structures are shown in **Figure 2**.

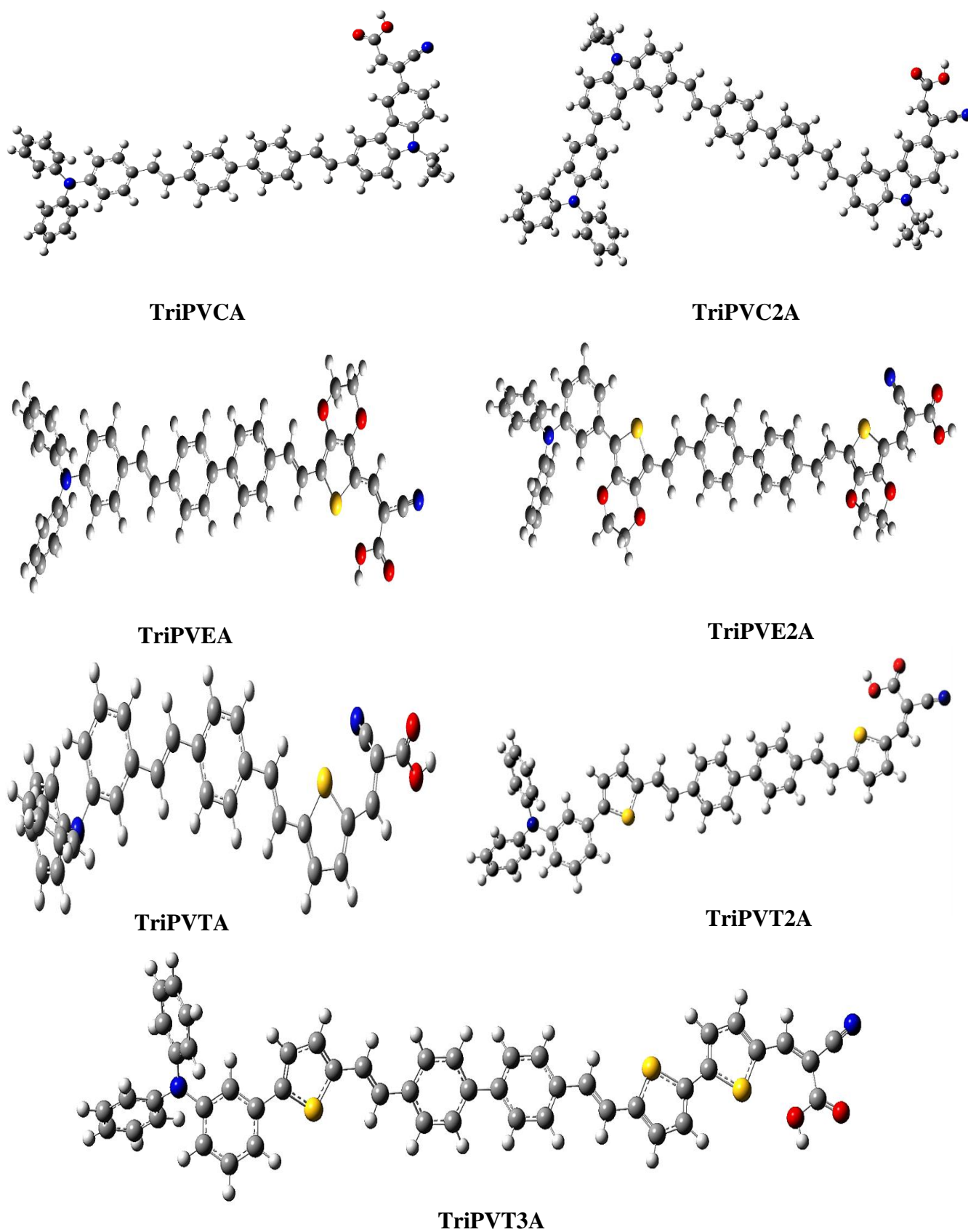


Figure 2. Optimized geometries for TriPVCA, TriPVC2A, TriPVEA, TriPVE2A, TriPVTA, TriPVT2A, and TriPVT3A obtained by B3LYP/6-31G (d,p) level of theory

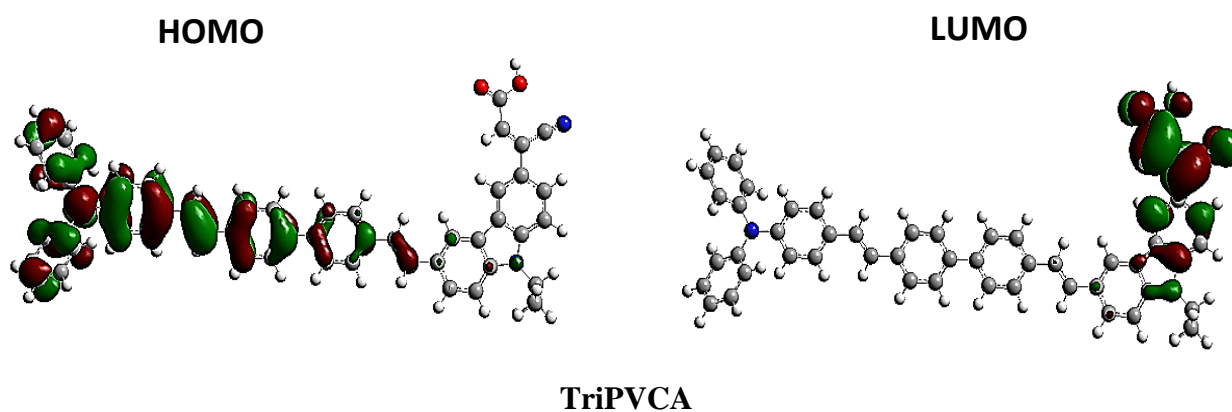
From these optimized geometries, we know that the conjugated bridges of the compounds are all planar. Indeed, the lengths are between 1.35 Å and 1.47 Å, and these values are between those of the single and double bonds of the carbon backbone (i.e., C-C: 1.530 Å, C=C: 1.339 Å N-C: 1.471 Å (Rittmeyer *et al.*, 2012, EL Malki *et al.*, 2017)). Thus, the conjugation present over the length of the whole system, and thus these values are the main cause of the shortening of the bond length, and thus the weakening of the π -conjugation. The dihedral angles and bond distance formed between Phenylenevinylene-Carbazole, Phenylenevinylene-Edot, or Phenylenevinylene-Thiophene groups as π -spacer group and the cyanoacrylic acceptor plane were presented in Table 1, the dihedral angles of all compounds are around 180°, hence the conjugated molecules are more planar. Therefore, it can be confirmed that the π -conjugated systems in these molecules should be more planar and thus the electron can be smoothly injected from the Triphenylamine donor to the cyanoacrylic acceptor.

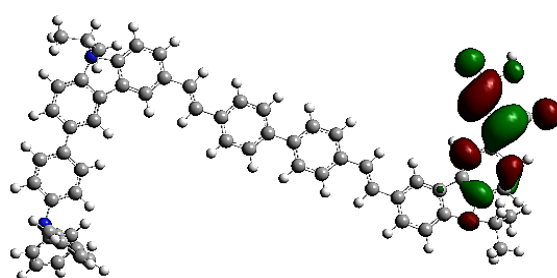
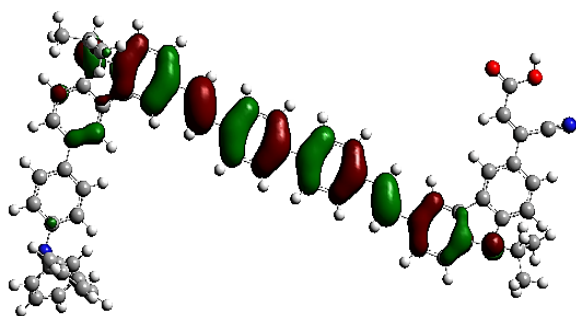
Table 1. Selected bond lengths and dihedral angles of optimized structures calculated by B3LYP/6-31G (d,p)

Compounds	Di (Å°)	Öi
TriPVCA	1.51	179.06°
TriPVC2A	1.42	179.97°
TriPVEA	1.54	180°
TriPVTE2A	1.48	179.75°
TriPVTa	1.41	177.38°
TriPVT2A	1.48	177.39°
TriPVT3A	1.428	179.93°

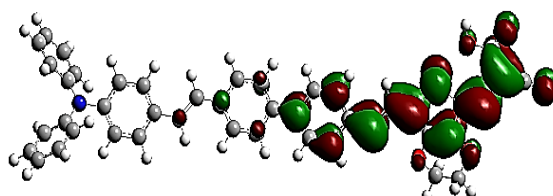
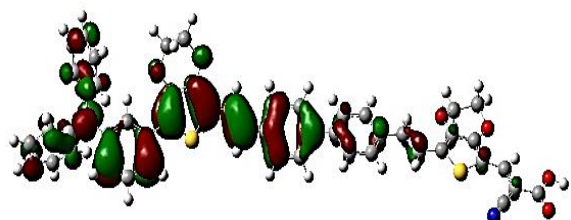
3.2 Frontier Molecular Orbitals

The investigation of the frontier molecular orbitals (FMO) has garnered considerable attention due to its ability to determine the separated charge states of studied compounds and facilitate efficient electron injection. This promotes electron transfer from the donor to the acceptor via the π -spacer (Pounraj *et al.*, 2018). In this study, we present the HOMO and LUMO electronic structures of seven molecules, as depicted in Figure 3, which demonstrate a high level of electron separation. The Triphenylamine-Phenylenevinylene donor units of the molecule backbone exhibit significant HOMO localization, while the bridges between subunits demonstrate significant LUMO delocalization, which indicates the flow of electron density. The electron density of LUMO is primarily localized on the 2-cyanoacrylic acid acceptor units. As a result, intramolecular charge transfer from the donor units to the anchor groups via the bridge likely accounts for the electronic transitions observed in the studied compounds, from HOMO to LUMO.

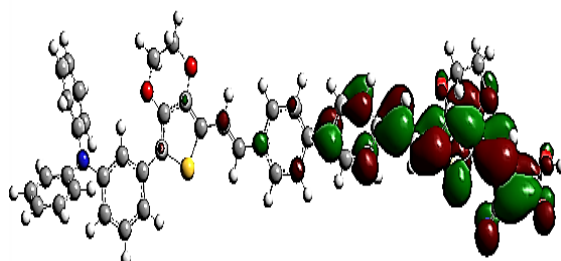
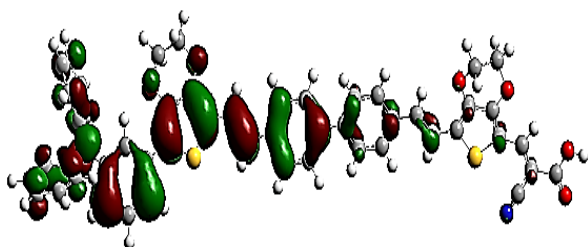




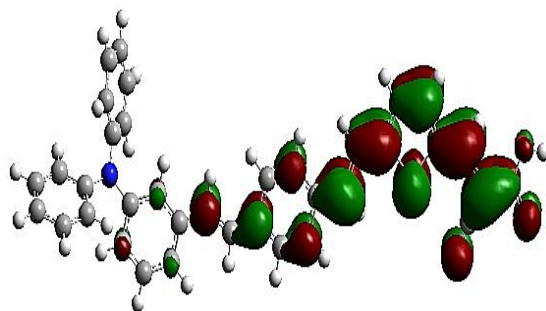
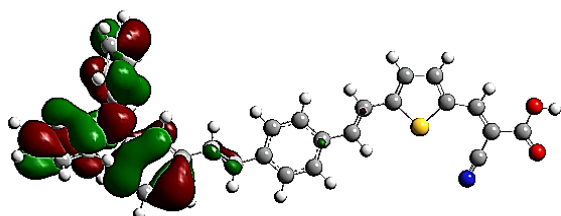
TriPVC2A



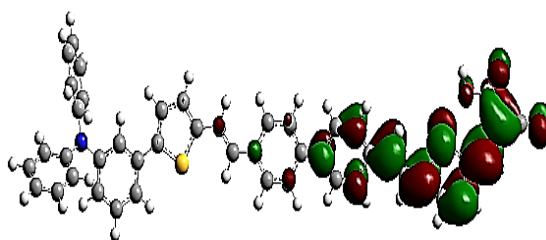
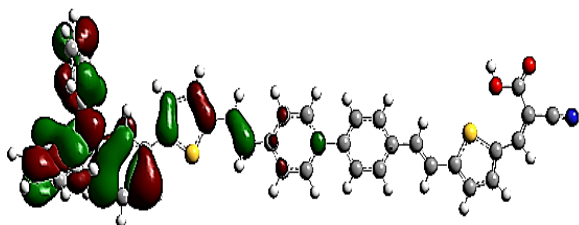
TriPVEA



TriPVE2A



TriPVTA



TriPVT2A

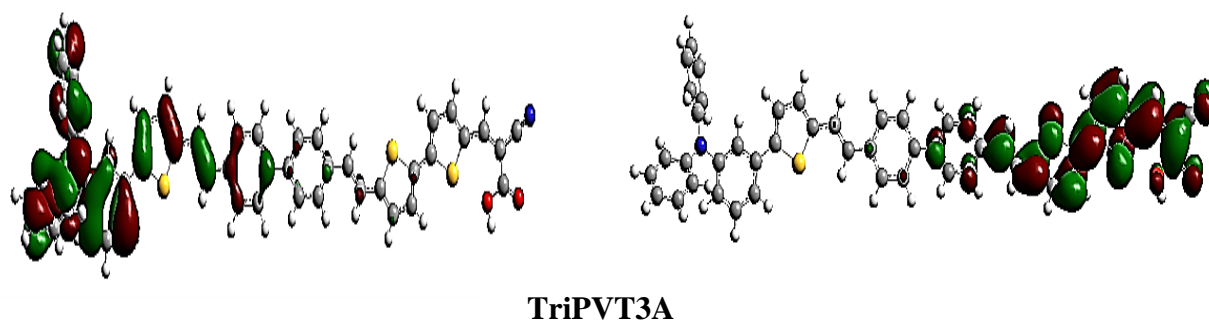


Figure 3. The contour plots of HOMO and LUMO orbitals of the studied compounds

3.3 Electronic properties

The electronic properties depend mainly on the energy levels of the most occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and the mobility of the electronic holes. Theoretical parameters related to the electronic properties (E_{HOMO} , E_{LUMO} , E_{gap} , V_{oc} , and α_i) are presented in [Table 2](#). The band gap (E_{gap}) of the studied molecules was obtained by the differences of HOMO and LUMO energy levels ($E_{\text{HOMO}} - E_{\text{LUMO}}$) using the B3LYP/6-31G (d,p) method. The E_{gap} energies of all compounds are between 2.15 eV and 2.38 eV in the following order: TriPVT3A < TriPVT2A < TriPVT1A < TriPVEA < TriPVE2A < TriPVC2A < TriPVCA. This order can be explained by the nature of the group and the π -conjugated length in the π -spacer part. We notice a decrease in the gap energy when we replace Carbazole and EDOT with Thiophene, this can be attributed to the higher electronegativity of the sulfur atom in thiophene, which leads to an increase in the conjugation length of the molecule, promising better TIC properties.

The difference between the theoretical and experimental results can be attributed to the fact that the calculations were carried out using an isolated molecule in gas phase to obtain the theoretical results and in solid phase to obtain the experimental results. [Table 3](#) presents an estimate of the E_{gap} value of the theoretical results obtained by DFT and the experimental results ([El Alamy et al., 2017](#)) of the two molecules TriPVT1A and TriPVT2A, we note a difference of 0.6 eV and 0.2 eV respectively. The authors specify that the estimated difference between experiment and theory in the case of conjugated systems is of the order of 0.2 eV ([Raftani et al., 2020](#)). Note that these results are in good agreement with the experimental work.

The maximum open circuit voltage (V_{oc}) is an important photovoltaic parameter that can be determined theoretically by the difference between the highest occupied molecular orbital (HOMO) of the molecule and the LUMO of the PCBM as an electron acceptor. Theoretical values of the open circuit V_{oc} have been calculated from the following expression ([Eqn.1](#)) ([Boussaidi et al., 2017](#)):

$$V_{\text{oc}} = E_{\text{HOMO}}^{\text{donor}} - E_{\text{LUMO}}^{\text{acceptor}} - 0.3 \quad \text{Eqn. 1}$$

Another parameter denoted α_i is determined by the difference between the LUMO energy levels of the molecules studied and the LUMO energy level of PCBM ([Eqn. 2](#)) ([Atmani et al., 2021](#)):

$$\alpha_i = E_{\text{LUMO}}^{\text{acceptor}} - E_{\text{HOMO}}^{\text{donor}} \quad \text{Eqn. 2}$$

Looking at [Table 2](#), we notice that all the values of V_{oc} are positive, which suggests that the electron transfers will be on the compounds to the PCBM acceptor, and for that we can say that these values are sufficient for a possible efficient electron injection.

As can be seen in **Table 2**, the obtained values of α_i are all positive, this indicates that all LUMO levels of all compounds are placed on the LUMO level of the PCBM, indeed, we infer that all compounds are susceptible to be injected into the excited state.

Table 2. The E_{HOMO} , E_{LUMO} , E_{gap} , and V_{oc} energies of the studied molecules obtained by B3LYP/6-31G (d,p)

Molecules	TriPVCA	TriPVC2A	TriPVEA	TriPVE2A	TriPVTA	TriPVT2A	TriPVT3A
E_{LUMO} (eV)	-2.40	-2.41	-2.67	-2.61	-2.84	-2.90	-2.93
E_{HOMO} (eV)	-4.78	-4.76	-4.92	-4.90	-5.10	-5.11	-5.08
E_{gap} (eV)	2.38	2.35	2.25	2.29	2.26	2.20	2.15
V_{oc} (eV)	0.58	0.56	0.72	0.70	0.90	0.91	0.88
α_i	1.5	1.9	1.23	1.29	1.06	1.00	0.97

Table 3. Theoretical and experimental Gap energy E_{gap} of TriPVTA and TriPVT2A

Compounds	$E_{\text{gap-exp}}$ (eV)	$E_{\text{gap-th}}$ (eV)
TriPVTA	2.10	2.26
TriPVT2A	2.00	2.20

The energy required to remove an electron from a neutral material can be specified by IP and the ability of the material to accept an electron from the environment is EA. In our study, we used IP and EA by the following relationships (**Eqn. 3**) (EL Karkri *et al.*, 2022) and (**Eqn. 4**) (El Alamy *et al.*, 2017):

$$\text{EA} = E(\text{M}) - E(\text{M}^-) \quad \text{Eqn. 3}$$

$$\text{IP} = E(\text{M}^+) - E(\text{M}) \quad \text{Eqn. 4}$$

Where $E(\text{M})$, $E(\text{M}^+)$ and $E(\text{M}^-)$ are the total energies of the neutral molecule, cation and anion states, respectively. We calculated the energies of the cationic states by removing one electron from the neutral molecule and the anionic states by adding one electron for each molecule at the B3LYP/6-31G (d,p) level while using the optimized geometry of the neutral form. The IP, EA are shown in **Table 4**. The calculated values of IP and EA for all molecules are between 5.30 eV and 6.12 eV and between 1.322 eV and 1.97 eV, respectively (see **Table 4**). Previous research has shown that increasing the LUMO energy level of these systems results in an increase in EA and leads to a higher value of V_{oc} (Qian *et al.*, 2015).

In order to assess the electron transfer potential of the molecules we studied to the conductive band of PCBM, an in-depth analysis of the HOMO (highest occupied level) and LUMO (lowest unoccupied level) levels was undertaken, as illustrated in **Figure 4**. This analysis plays a crucial role in understanding the mechanisms underlying the photovoltaic performance of organic cells. Crucially, the LUMO energy levels of the molecules studied are at energy levels above the ITO conduction band (-4.7 eV). This observation is significant: it indicates that molecules, when in excited states, hold a considerable capacity to inject electrons towards ITO electrodes. This property is essential for efficient current generation and collection in organic photovoltaic cells. Furthermore, it is remarkable that the HOMO and LUMO levels of the molecules studied correlate perfectly with the requirements of a high-performance photosensitizer. More specifically, the LUMO levels of these molecules surpass those of PCBM. This characteristic confers considerable driving forces, creating an environment conducive to effective and efficient electron injection.

In sum, these findings suggest that the molecules we have examined hold promising potential as sensitizers in the context of organic solar devices. By facilitating the process of injecting electrons from these molecules into the conduction band of the PCBM and enabling subsequent regeneration.

Table 4. The molecular properties EA (eV), and IP (eV), of the studied compounds obtained by B3LYP/6-31G(d,p) level

Molecules	TriPVEA	TriPVE2A	TriPVCA	TriPVC2A	TriPVTA	TriPVT2A	TriPVT3A
EA	1.72	1.697	1,322	1.47	1,811	1.90	1.97
IP	5.78	5.70	5.62	5.30	6.12	5.98	5.87

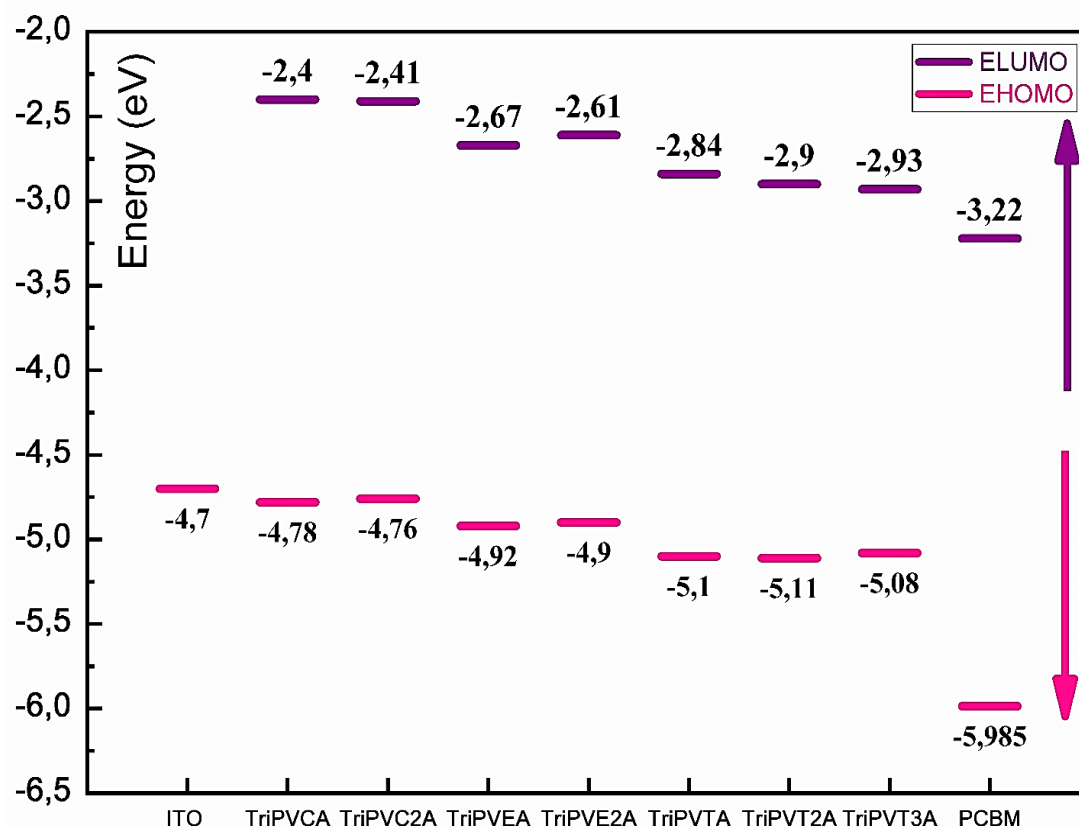


Figure 4. Sketch of calculated energy levels of the HOMO and LUMO for the studied compounds and the PCBM

3.4 UV/Vis absorption spectra

How well the absorption of a new material matches the solar spectrum is an important factor for application as a photovoltaic material, and a good photovoltaic material should have broad and strong absorption characteristics in the visible. The longest wavelength of the UV-Visible spectra of the tested compounds from the optimized structures are calculated by the TD-DFT method (**Figure 5**), the values of λ_{max} located at the electronic transition from HOMO-1 to LUMO of the seven compounds are in the following order: TriPVT3A (613.45nm) > TriPVTA (607.35nm) > TriPVT2A (600.02nm) > TriPVEA(597.93nm) > TriPVE2A (587.81nm) > TriPVC2A (562.99nm) > TriPVCA (558.97nm). All the studied compounds show a simulated wavy absorption spectrum; this may be due to the increase in the length of π -conjugation which can enhance the light capture ability of a photosensitive component, and the intermolecular band transfer charge caused by the acceptor unit introduced in the structures of these molecules, resulting in broader absorption bands. Thus, the maximum absorption wavelength is

that of thiophene which can be explained by the strong electron donation of thiophene. Thus, these organic materials could absorb the maximum incident light radiation, and the energy range classified in the UV range for all structures.

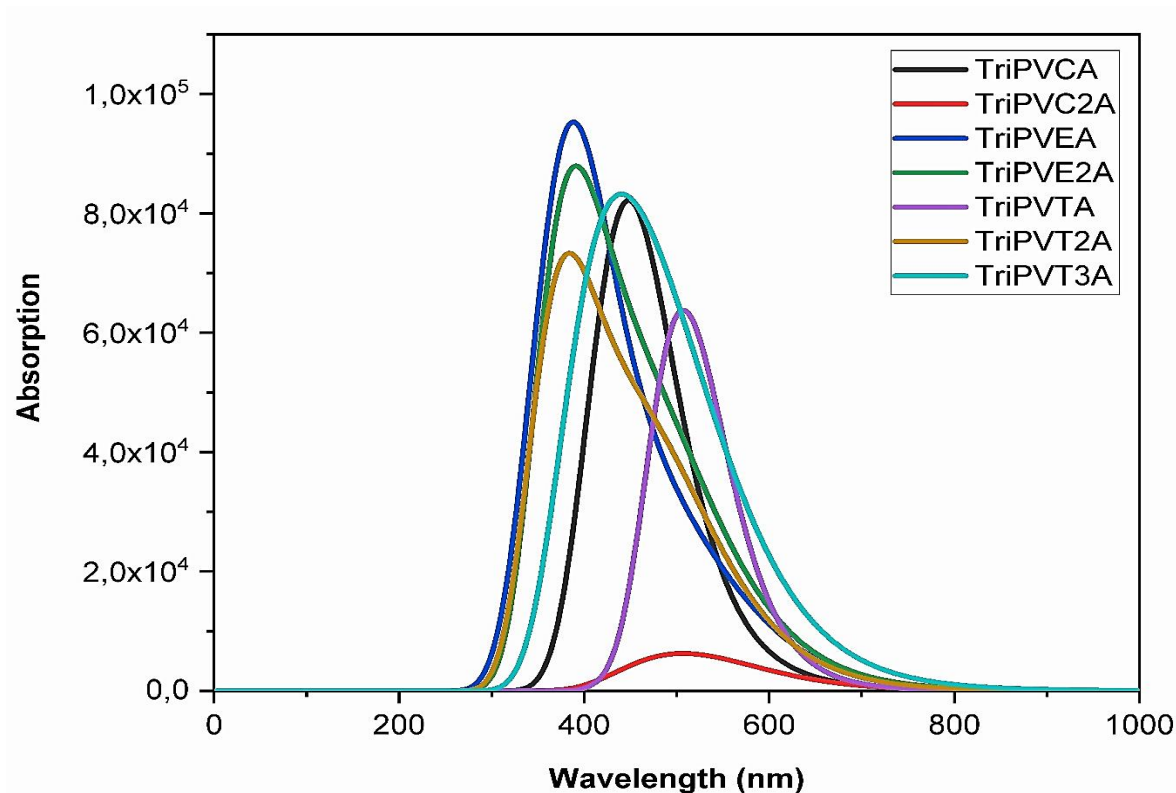


Figure 5. Simulated UV-Visible optical absorption spectra of the studied compounds calculated by TD-DFT/B3LYP/6-31G (d, p) level

3.5 Photovoltaic properties

3.5.1 Parameters of organic solar cells

The plot of the current-voltage characteristic allows access to multiple physical parameters of the component. The first parameters that appear on the current-voltage characteristic of a photovoltaic cell are the short-circuit current density (J_{sc}), the open-circuit voltage (V_{oc}), the filling factor (FF) of the component and the power conversion efficiency (PCE).

i. The short-circuit current density (J_{sc})

This is the highest current density that can be obtained with a solar cell. It increases linearly with the illumination intensity of the cell and depends on the illuminated surface, the wavelength of the radiation, the mobility of the carriers and the temperature (Mhamedi *et al.*, 2022).

ii. The fill factor FF

The fill factor FF reflects the degree of ideality of the $J(V)$ curves. It is determined by the following equation (Eqn. 5) (Scharber *et al.*, 2006):

$$FF = \frac{P_{max}}{V_{oc} \cdot J_{sc}} = V_{max} \cdot \frac{J_{max}}{V_{oc} \cdot J_{sc}} \quad \text{Eqn. 5}$$

Where J_{max} and V_{max} respectively represent the current density and voltage of the operating point that allows to extract the maximum power (P_{max}) of the cell. From The fill factor, it is possible to obtain information on the quality of the material–electrode interfaces.

iii. The power conversion efficiency

The power conversion efficiency of photovoltaic cells is defined as the ratio between the maximum power P_{\max} delivered by the cell and the incident light power, P_{in} (Eqn. 6) (Bourass *et al.*, 2013):

$$\eta = \frac{FF \cdot V_{OC} \cdot J_{SC}}{P_{in}} \quad \text{Eqn. 6}$$

iv. Series R_s and shunt R_{sh} resistances

The series resistance R_s characterizes the voltage losses in the semiconductor and through the ohmic contacts of the cell. It takes into account the resistivity of the material, of the electrodes and of the semiconductor-metal contact.

The shunt resistance R_{sh} reflects the presence of a leakage current in the diode due to the recombination of carriers in the vicinity of the charge dissociation sites (at the D/A interface and at the electrodes) and to the possible existence of a leakage initiated by the geometric inhomogeneities of the layers (El Karkri *et al.*, 2020).

- The slope of the curve $J(V)$ at point V_{oc} represents the inverse of the series resistance $1/R_s$.
- The slope of the curve $J(V)$ at point J_{sc} represents the inverse of the shunt resistance $1/R_{sh}$.

3.5.2 Studied structure

In this part of the work, we will focus our efforts on the characterization of a bulk heterojunction organic photovoltaic cell between the studied molecules and the PCBM acceptor. The chosen structure is shown in Figure 6.

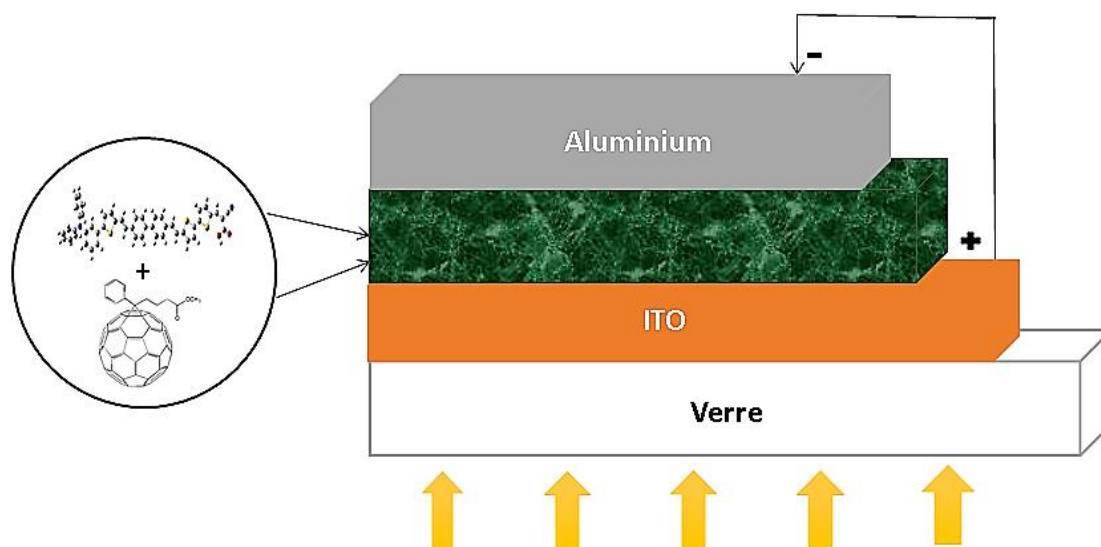


Figure 6. Organic photovoltaic cell studied

3.5.3 Current-voltage characteristics

The photovoltaic properties of the seven oligomers with PCBM acceptor were studied by AMPS-1D. At room temperature (300 K) and under an illumination of 300 mW/cm², Figure 7 illustrates the current-voltage traits of the examined cell for all compounds. The Open circuit voltage (V_{oc}), short circuit current density (J_{sc}), form factor (FF), power conversion efficiency (η), The series resistance R_s , and the shunt resistance R_{sh} obtained from the simulation are listed in Table 5.

The V_{oc} values of all compounds TriPVCA, TriPVC2A, TriPVEA, TriPVE2A, TriPVTA, TriPVT2A, TriPVT3A are 0.668 eV, 0.694 eV 0.75 eV 0.809 eV, 0.88 eV, 0.94 eV, 0.99 eV respectively, which are in agreement with the simulated values by DFT. The TriPVT3A showed a simulated PCE (power conversion efficiency) value of 8.58% with a J_{sc} of 10.644 mA/cm² and a FF of 0.808. The TriPVT2A showed a simulated PCE (power conversion efficiency) value of 8.09% with a J_{sc} of 10.644 mA/cm² and a FF of 0.801. The TriPVTA showed a simulated PCE (power conversion efficiency) value of 7.41% with a J_{sc} of 10.641mA/cm² and a FF of 0.789. The TriPVE2A showed a simulated PCE (power conversion efficiency) value of 7.59% with a J_{sc} of 11.606mA/cm² and a FF of 0.809.

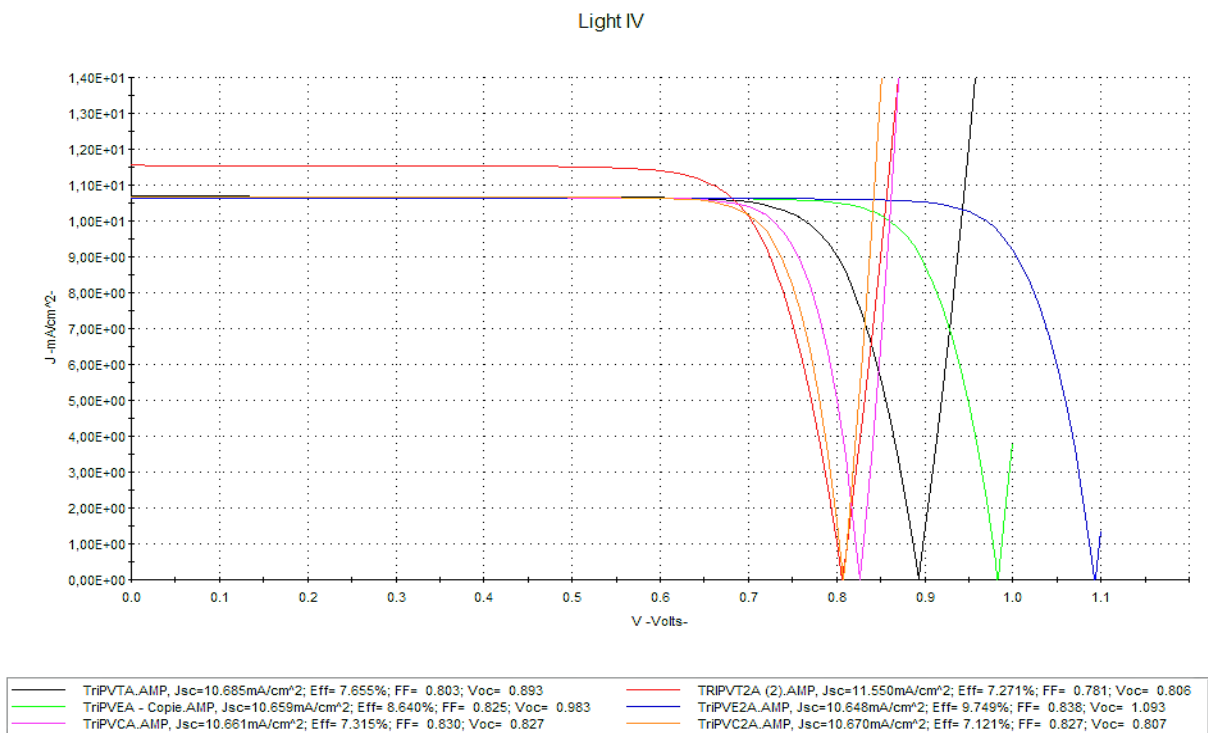


Figure 7. Current-voltage characteristics

Table 5. Characterization of photovoltaic parameters in organic cells of the compounds studied obtained by AMP1D

Molecules	TriPVCA	TriPVC2A	TriPVEA	TriPVE2A	TriPVTA	TriPVT2A	TriPVT3A
V_{oc} (eV)	0.668	0.694	0.75	0.809	0.88	0.94	0.99
J_{sc} (mA/cm ²)	13.90	11.683	10.758	11.606	10.641	10.644	10.644
FF	0.746	0.768	0.787	0.809	0.789	0.801	0.808
$\eta\%$	6.93	6.23	6.35	7.59	7.41	8.09	8.58
R_s (Ω cm ²)	3.60	4.90	5.50	5.30	9.40	5.70	6.70
R_{sh} (Ω cm ²)	77.14	78.59	96.98	102.42	98.86	156.77	137.43

The TriPVEA showed a simulated PCE (power conversion efficiency) value of 6.35% with a J_{sc} of 10.758 mA/cm² and a FF of 0.787. The TriPVC2A showed a simulated PCE (power conversion efficiency) value of 6.23% with a J_{sc} of 11.683 mA/cm² and a FF of 0.768. The TriPVCA showed a simulated PCE (power conversion efficiency) value of 6.93% with a J_{sc} of 13.906 mA/cm² and a FF of

0.746. The efficiency increased to a value of 8.58% for TriPVT3A, due to the addition of the thiophene unit. We found an increase in the efficiency value compared to other literature results, such as poly(3-hexylthiophene) (P3HT). To minimize the losses, R_s must be decreased and R_{sh} increased. A zero series resistance and a shunt resistance equal to infinity (El Karkri *et al.*, 2022; Arbouch *et al.*, 2014) characterize an ideal photovoltaic cell.

Conclusion

We used DFT/TD-DFT to design and investigate by quantum simulation the structural, optoelectronic and optical properties, as well as photovoltaic parameters of a series of low band gap donor- π -acceptor conjugated molecules bearing the Triphenylamine-Phenylenevinylene unit and different donor units consisting of (3, 4 Ethylenedioxythiophene) (Edot), carbazole and thiophene. Our results show that the designed compounds can serve as organic BHJ solar cells, as their LUMO energy levels are higher than PCBM. The V_{oc} and α_i parameters are positive, suggesting that electron transfers will occur on the compounds to the PCBM acceptor. Their PCE power conversion efficiency ranges from 6.23% to 8.58%. Furthermore, the optimized geometries revealed that the conjugated bridges of the compounds are planar, thus favoring electron injection from the Triphenylamine donor to the cyanoacrylic acid acceptor. The electron density of the most occupied molecular orbitals (HOMO) is mainly localized on the Triphenylamine-Phenylenevinylene donor moiety, while the electron density of the least occupied molecular orbitals (LUMO) is extended on the acid groups of the acceptor. The localized λ_{max} values of the seven compounds show broad absorption characteristics in the visible range. These results suggest that the investigated materials could be good candidates for applications in organic solar cells.

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