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Photovoltaic Energy Conversion and Optical Properties of Organic Molecules Based on Aceanthraquinoxaline

Taoufik Sahdane*, Bousselham Kabouchi, Abbes Laghrabli, Brahim Azize

Molecular Spectronomy, Optics and Laser Instrumentation Team, Mohammed V University in Rabat, Agdal, Rabat, Morocco

ABSTRACT

In this investigation, we out theoretical study of electronic properties and geometry of four conjugated molecules based on aceanthraquinoxaline are used as donor layer for organic thin-film solar cells. The impact the substituted groups on the optoelectronic and structural properties, dipole moment, Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO) and gap energies (Egap) are argue. The geometry at the ground state and the electronic structure of studied molecules are procure by Density Functional Theory (DFT) and density functional theory time-dependent (TD-DFT) with the B3LYP/6-31G (d). The results of this study exhibit that these compounds are good candidates for organic solar cells.

Keywords: Aceanthraquinoxaline, Electronic properties, DFT, HOMO, LUMO, Photovoltaic, Organic solar cells

INTRODUCTION

Solar panels on silicon are currently the most popular; this technology is limited by its high cost. An emerging technology that can address the current gaps in the field is organic photovoltaics in which semiconductors are carbon-based. These compounds are much less expensive to manufacture and require a lower initial investment [1,2]. They also exhibit the ability to be dissolved and incorporated into inks. They may benefit from the enormous expertise in printing technology, low cost and high speed of production. In addition, organic devices can be fabricated on flexible or semi-transparent substrates, and can benefit from new applications, such as solar textiles that wrap for easy transport, solar tinted windows [3,4]. The main limitation of organic photovoltaics is its low efficacy compared to its inorganic counterparts. To be economically viable and competitive, it is crucial to increase this effectiveness. To do this, we need to find organic compounds, which have the most relevant electronic properties, including optimum band gap and energy levels allowing heterojunction effective. The synthesis of all compounds is completely impossible, and it is crucial to probe how the theoretical properties for better effectiveness. Scharber et al. proposed a semi-empirical model in 2006 to explain the operation of the organic devices and provide an efficiency maximum of 11% based on this model [5]. It is useful from first principles and solving the Schrödinger equation. These calculation methods that are not based on experimental data are called *ab-initio*. An interesting technique to resolve the Schrödinger equation is the density functional theory [6].

Organic semiconductors have attracted the regard of researcher's theorists and experimentalists in recent years, due to their excellent optical and electronic properties [7]. These materials can be used for producing such diverse devices as photovoltaic cells, field effect transistors, and light emitting diodes [8-13]. Most research of new conjugated molecules with specific applications has be one of the attractive topics in the fields of physical and chemical materials [14]. A necessary understanding of the relationship between structure and properties of these materials is desired to exploit their properties for photovoltaic cells.

In this study, four compounds based on aceanthraquinoxaline (AQ_1, AQ_2, AQ_3, AQ_4) are considered. These compounds were studied using DFT and TD-DFT calculations. HOMO, LUMO, Egap and open circuit voltage (V_{oc}) of all molecules are investigated (Figure 1).

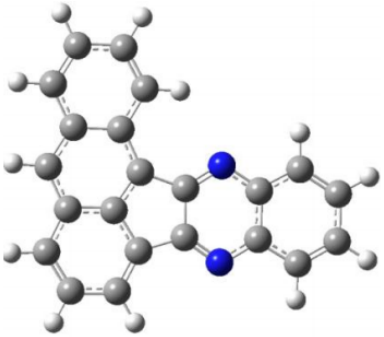

Figure 1: Structure of aceanthraquinoxaline (AQ_1)

MATERIALS AND METHODS

The calculations are take-out using the program GAUSSIAN 03 [15], and the simulation of current-voltage (J-V) characteristics, fill factor, open-circuit voltage, and conversion efficiency of organic photovoltaic cell was well established by gpvdm software. The geometry optimization of the studied compounds is evaluated by DFT/B3LYP using 6-31G (d) basis set [16]. The electronic absorption spectra are exploring using TD-DFT calculations with B3LYP/6-31G (d).

The circuit diagram has been given in Figure 2 [17].

Materials used for the design and bandwidth values data of materials are given in Table 1.

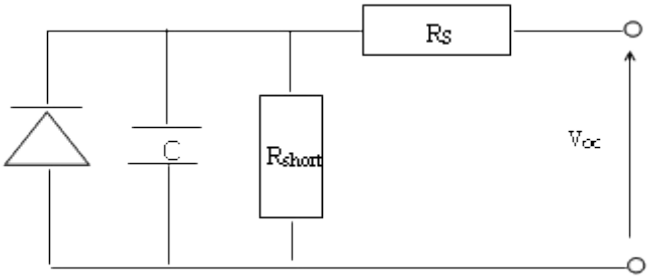

Figure 2: Equivalent circuit of organic solar cell

Table 1: Two-layer organic photovoltaic cell

ITO (electrode 1) 100 nm
aceanthraquinoxaline (donor)
PCBM (acceptor) 100 nm
Al (electrode 2) 100 nm

RESULTS AND DISCUSSION

In organic solar cells, the open circuit voltage (Voc) is found to be linearly depending on the HOMO donor and LUMO acceptor energies which are important factors in determining that effective charge transfer will occur between the donor and acceptor.

The power conversion efficiency (PCE) can be got using the following equation:

$$PCE = \frac{FF.V_{OC}.J_{SC}}{P_{in}}$$

Where FF is the fill factor, J_{sc} is the short circuit current and P_{in} is the incident power density.

The optimized molecular structures are depicted in Figure 3. Table 2 exhibits the calculated orbital energies and energy gap between HOMO and LUMO. Figure 4 shows the characteristics of the AQ_1/PCBM solar cells under various light intensities.

Table 2: Energy values of LUMO, HOMO, and Egap of the studied molecules obtained by B3LYP/6-31G (d)

Compound	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{gap} (eV)
AQ_1	-6.61	-2.39	4.22
AQ_2	-5.88	-2.37	3.51
AQ_3	-7.22	-2.87	4.35
AQ_4	-6.76	-2.45	4.31

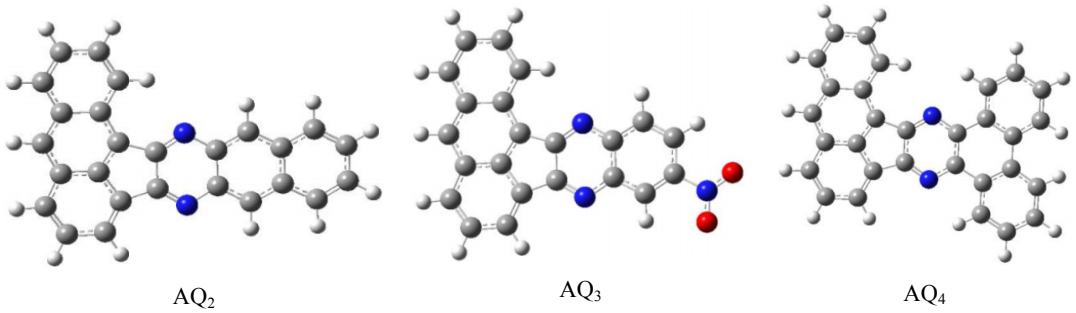

Figure 3: Optimized molecular structures computed by DFT/B3LYP/6-31 G(d)

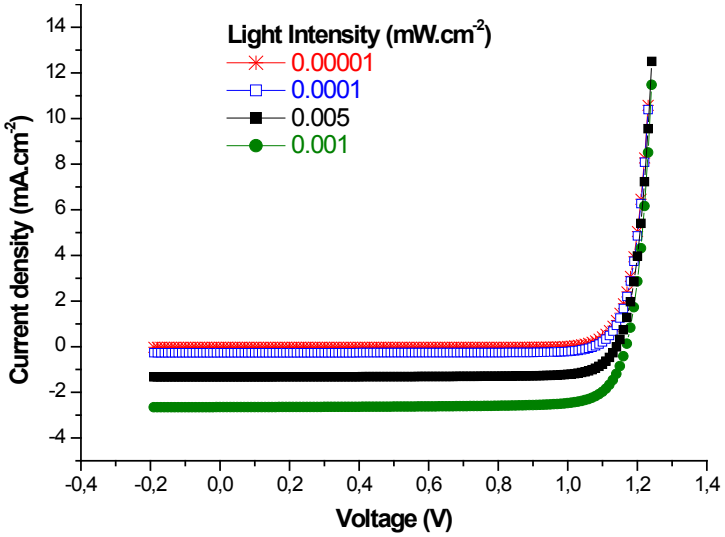

Figure 4: J-V characteristics of AQ_1/PCBM solar cells under various light intensities (Layer thickness AQ_1=100 nm)

Figure 5 shows the characteristics of the AQ_1/PCBM solar cells under various layer thicknesses AQ_1.

In Figure 6, we plotted the electron spatial distribution of HOMO and LUMO orbitals of all compounds. The HOMO and LUMO demonstrated the typical π-type molecular orbital characteristics.

As view in Table 3, we can get the values of wavelengths λ_{max} calculated and oscillator strengths (f). Excitation state S1 tie in almost exclusively to the allocation of an electron from the orbital HOMO of LUMO. The wavelengths of absorption wave ensue from electronic transition S0→S1 that increases progressively with the increase of conjugation lengths. It is reasonable, the transition between HOMO→LUMO is predominant in S0→S1 electronic transition, and the consequent are a decrease of LUMO and an increase of HOMO energy.

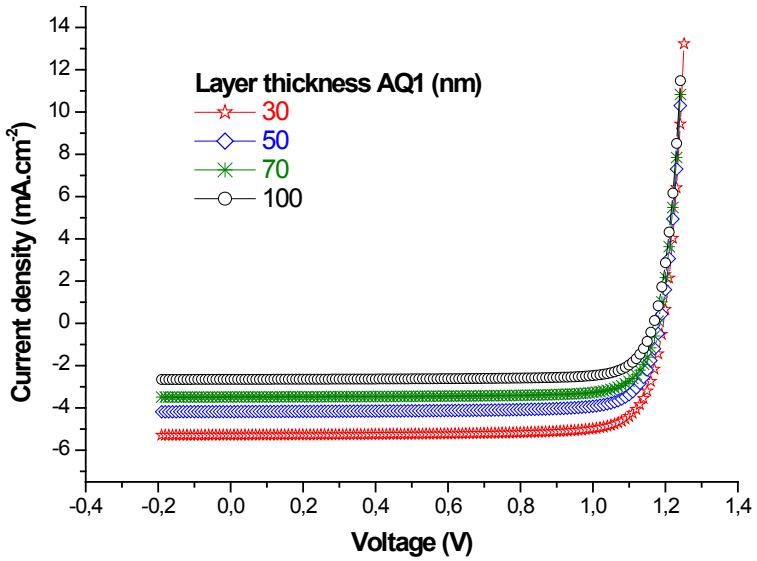

Figure 5: J-V characteristics of AQ_1/PCBM solar cells under various layer thickness of AQ_1 (Light intensity=0.001 mW.cm^{-2})

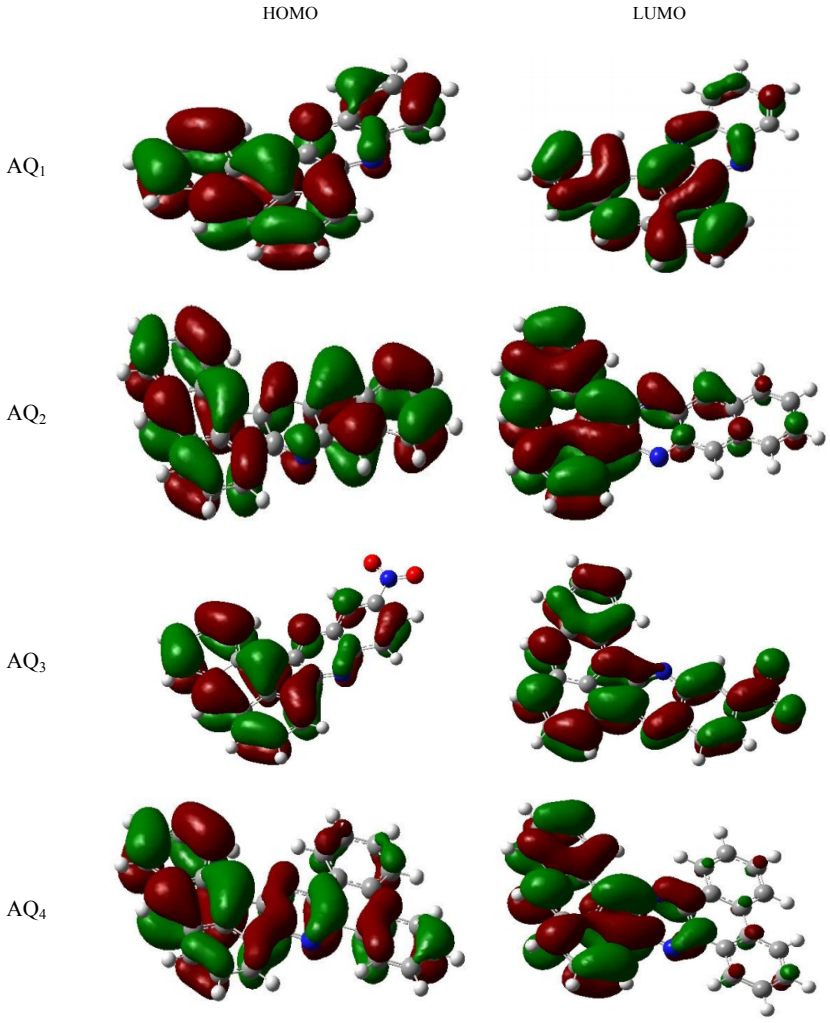

Figure 6: Obtained isodensity plots of the frontier orbital HOMO and LUMO of the studied compounds obtained at B3LYP/6-31(d) level

Table 3: Absorption spectra data obtained by TD-DFT methods for compounds at B3LYP/6-31G (d) optimized geometries

Compound	λ_{max} (nm)	$E_{activation}$ (eV)	f	MO/character
AQ_1	423.66	79.689	0.43	HOMO->LUMO (93%)
AQ_2	429.86	78.539	0.522	HOMO->LUMO (91%)
AQ_3	436.12	77.412	0.624	HOMO->LUMO (87%)
AQ_4	445.19	75.836	0.334	HOMO->LUMO (93%)

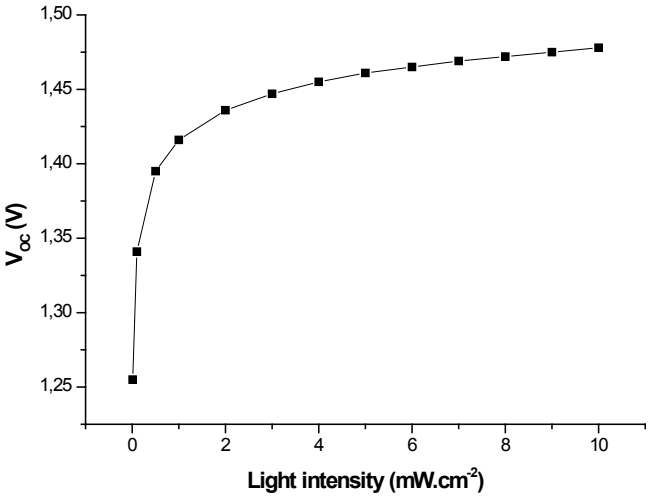

Figure 7: Influence of light intensity on open circuit voltage (V_{OC}) of AQ_1/PCBM solar cells (Layer thickness AQ_1=100 nm)

Since all the compounds (AQ_1, AQ_2, AQ_3, AQ_4) thus almost the same behavior, we present in the following the results corresponding to AQ_1.

The V_{OC} is allied to the light intensity. On this root, we have established a simulation for the relationship between the V_{OC} and the light intensity, as shown in Figure 7.

Figure 8 shows the effect of light intensity on the fill factor (FF). FF decreases when the light intensity increases.

The impact of layer thickness AQ_1 on short-circuits density (J_{SC}), open-circuit voltage (V_{OC}), fill factor (FF), and conversion efficiency (PCE) is given in Table 4.

The percent efficiency is mainly affected by the light intensity. The results shown in Figure 9, with the light intensity increase, percent efficiency decreases.

Table 4: Electrical parameters of the AQ_1/PCBM solar cells with layer thickness AQ_1

Layer thickness AQ_1 (nm)	J_{SC} (mA.cm^{-2})	V_{OC} (V)	FF (%)	PCE (%)
30	1.664	1.194	80.079	15.913
50	1.315	1.185	80.061	12.474
70	1.096	1.178	80.29	10.375
100	0.835	1.168	80.207	7.817
150	0.495	1.147	80.645	4.581
200	0.29	1.125	80.629	2.628
300	0.108	1.085	81.124	0.949

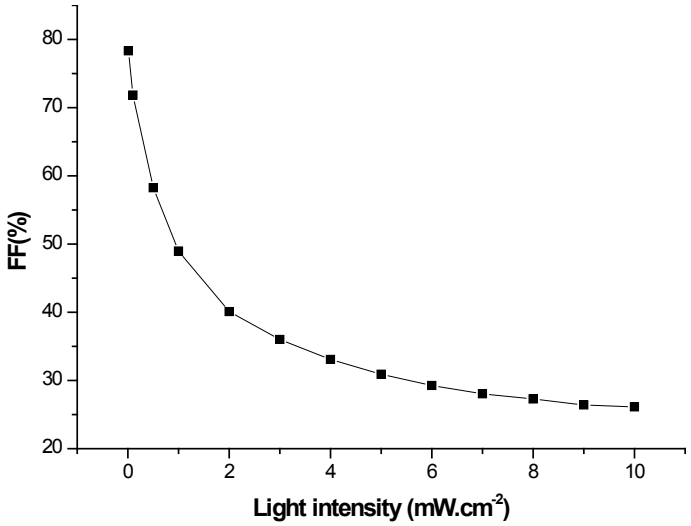

Figure 8: Influence of light intensity on fill factor (FF) of AQ_1/PCBM solar cells (Layer thickness AQ_1=100 nm)

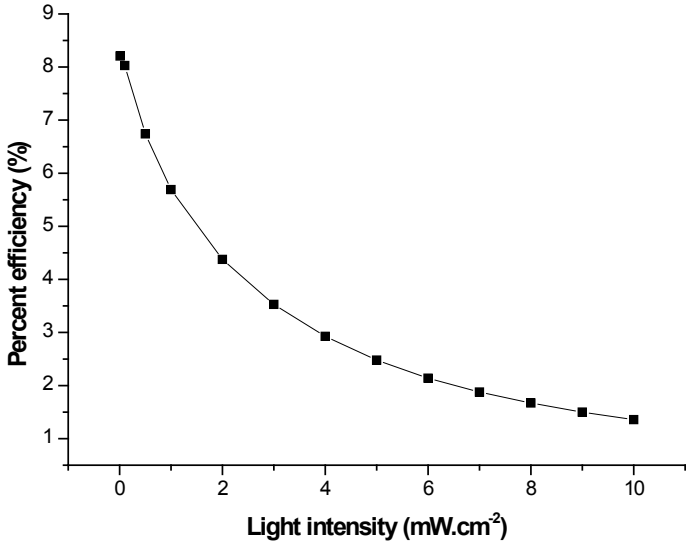

Figure 9: Influence of light intensity on percent efficiency of AQ_1/PCBM solar cells (Layer thickness AQ_1=100 nm)

CONCLUSION

In this paper, the properties of the optical absorption and electronic structure of four compounds based on aceanthraquinoxaline were studied employing DFT and TD-DFT methods. We conclude the changes of several donors or acceptor groups do not change the geometric parameters and the energies of the orbital HOMO, LUMO and Egap showed that Egap studied molecules differ from 3.51-4.35 eV for the different structures. From these results, we can conclude that these compounds have shown significant optoelectronic properties, which leads to offer these materials for application of organic solar cells. This calculation process can be used as a model system for understanding the relationship between the electronic properties and molecular structure and can as be used to study their aptitude in electroluminescent devices. The results propose these materials as candidate for organic solar cells.

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