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A first principle study of benzimidazobenzophenanthrolin and tetraphenyldibenzoperiflanthene to design and construct novel organic solar cells

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ABSTRACT

In this study, through DFT and TDDFT computational methods and by using benzimidazobenzophenanthroline (BBL) as an acceptor and tetraphenyldibenzoperiflanthene (DBP) as a donor, a Donor-Acceptor (D-A) system was devised on the purpose of designing and simulating organic solar cells. The optimization of this system was done in the basic state using the basis set and the method of B3LYP/6-311 + G*. The energy of HOMO and LUMO orbitals and the electron localization function (ELF) were also investigated. The LUMO orbital energy of the acceptor (A) was 0.51 eV less than that of the donor (D), which is close to the ideal value. The computation of the excited state was performed by using the CAM-B3LYP method and the same basis set. The hole-electron theory implemented in the excited state visually proved a charge transfer (CT) for the D-A system, which was based on the computations in the ground state. Typically, organic solar cells have a CT at one wavelength. The CT results show that there are two considerable CTs at 356- and 487-nm wavelengths, indicating the acceptable efficiency of this system.

1. Introduction

Nowadays, because of the importance of new sources of energy, production of materials which are able to generate electrical energy has come into focus [1]. Sunlight is one of the natural resources that can be converted to electrical energy using photovoltaic cells [2]. So, in recent years, light-sensitive materials applied in these cells have been the topic of a lot of research [3,4]. Indeed, the new generation of solar cells is based on organic compounds that have attracted the attention of researchers by virtue of their various advantages. The significant characteristics of organic solar cells include low cost, light weight, and ease of construction [5]. Their solubility in organic solvents enhances their importance and makes it possible to provide flexible solar cells [6].

Organic solar cells have specific characteristics. Because the active materials used in the production of solar cells are soluble in many organic solvents, polymeric solar cells have the necessary flexibility as well as the capability of being constructed in a continuous printing process, such as the process in newspaper publication [7,8]. One of the important parameters which should be considered during the designing of organic solar cells is the suitable selection of an electron donor and an electron acceptor for such systems. The donor must have the ability of charge transfer to an acceptor in an excited state, for which conjugated polymers are usually used [9,10]. These polymers are recently taken into consideration for their practical capabilities in flexible electronic instruments such as LEDs, polymer solar cells, and thin-layer organic transistors as well as their low price and ease of processing in solutions [7,11,12]. What is important about polymer solar cells is the improvement of their efficiency and light absorption rate and production of new structures with multiple morphologies, increased flexibility and environmental stability. In general, polymer materials which have π electrons can produce an electrical charge by absorbing sunlight; therefore, these materials have the capability of being used in polymer solar cells [12,13]. Most semi-conductive polymers are hole transmitters, which are known as donor polymers. Benzimidazobenzophenanthroline (BBL) is an acceptor with a high capability of being widely used in designing and constructing solar cells [10,14].

Paying attention to the energy level of D LUMO and A orbitals is the strategy used in the selection of donors and acceptors for organic solar cells. The highest efficiency belongs to the cells in which the LUMO energy level of A has a maximum value of 0.5eV or less than that of D. Based

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on the type of the system, the donor and the acceptor can be separated or connected together [15]. Organic acceptors have a wide diversity and are selected based on the type of donors and the system of organic solar cells. An interesting acceptor is the one with metallic bond capability [16,17]. Indeed, a major advantage of such an acceptor is its easy attachment to electrodes. Considering its special electronic characteristics, a tetraphenyldibenzoperiflanthene (DBP) [18]compound has been used as an acceptor along with strong donors, such as alpha-sexithiophene, and as a donor along with strong acceptors, such as C_{60} [19,20].

In this study, DFT and TDDFT computational methods are used to investigate a donor-acceptor system for its potential to be applied in organic solar cells [21–25]. A DBP combination and a BBL combination are used as a donor and an acceptor respectively (Fig. 1). Because of the lower level of LUMO in the BBL combination than in the DBP combination, the former combination serves as a strong acceptor.

2. Methodology

DBP, BBL and the D-A system, presented in Fig. 1, were optimized in the ground state by using the DFT method with a B3LYP function and a 6-311 + G* basis set. It is to be noted that the energy level of the HOMO and LUMO orbitals of donors and acceptors serves as one the most important parameters in designing and constructing organic solar cells. The DOS (density of states) graphs were obtained in the ground state. Generally, such graphs present a good image of the energy gap between HOMO and LUMO orbitals, and investigation of them is necessary for electronic and semi-conductive systems, such as transistors and solar cells [26–29]. An analysis of the Natural Bond Orbitals (NBO) performed through the same method in the ground state determined the charge details of the D-A system. The results are provided in Table 2 [30].

ELF is a suitable visual parameter for electronic density investigations. The parameter, in fact, shows the possibility of electron existence in the vicinity of reference electrons with the same spin. ELF clearly separates the electrons of the valance band and the core layer, which is helpful for comparing the performances of acceptors [31–33].

In this study, all the computations were performed in an excited state by using the TDDFT method with a CAM-B3LYP function and a basis set of 6-311 + G* [34,35]. To investigate the performance of the charge transfer (CT) in the donor-acceptor (D-A) systems, the hole-electron theory was used. This theory has a proper approximation and can calculate the length of the charge transfer and determine the overlap integral of electrons and hole orbitals [28]. The longer the charge-transfer is, the better the performance of the D-A system. Using Gaussian 03 software [36], all the calculations were done in a gas phase and under the environment pressure. Also, Multiwfn [37] and Gaussum [38] software programs were used for the analysis of some results.

Table 1
NBO analysis of the D→A system and A→D in the D-A system.

D→A		A→D	
$\pi C_{1}\text{-}C_{6}\rightarrow\sigma^{*}\ C_{127}\text{—}H_{139}$	1.02	$\pi C_{115}\text{-}C_{116}\rightarrow\sigma^{*}\ C_{13}\text{—}H_{169}$	0.87
$\sigma\ C_{18}\text{—}H_{20}\rightarrow\ \sigma^{*}\ C_{123}\text{—}O_{125}$	0.08	$\pi C_{118}\text{-}C_{119}\rightarrow\pi^{*}\ C_{7}\text{—}O_{8}$	0.15
$\sigma\ C_{18}\text{—}H_{20}\rightarrow\ \pi^{*}\ C_{123}\text{—}O_{125}$	0.023	$\pi C_{123}\text{-}O_{125}\rightarrow\pi^{*}\ C_{18}\text{—}O_{74}$	2.46
$\pi\ C_{26}\text{—}C_{27}\rightarrow\ \pi\ C_{113}\text{—}O_{124}$	0.27	LP $O_{125}\rightarrow\sigma^{*}\ C_{18}\text{—}H_{74}$	3.24
$\pi\ C_{29}\text{—}C_{30}\rightarrow\ \pi^{*}\ C_{112}\text{—}C_{120}$	0.30	LP $O_{125}\rightarrow\sigma^{*}\ C_{18}\text{—}H_{74}$	0.71
$\pi\ C_{29}\text{—}C_{30}\rightarrow\ \pi^{*}\ C_{118}\text{—}C_{119}$	0.39	LP $N_{125}\rightarrow\sigma^{*}\ C_{13}\text{—}H_{169}$	0.71
$\pi\ C_{56}\text{—}C_{57}\rightarrow\ \sigma^{*}\ C_{129}\text{—}O_{143}$	0.24		

Table 2
NBO analysis of internal transmissions A in the presence and absence of D.

A	Without complex	Complex
LP $O_{125}\rightarrow\sigma^{*}\ C_{118}\text{—}O_{123}$	2.45	2.69
LP $O_{125}\rightarrow\sigma^{*}\ N_{122}\text{—}O_{123}$	1.53	1.20
LP $N_{126}\rightarrow\sigma^{*}\ C_{116}\text{—}O_{121}$	3.47	3.27
LP $N_{126}\rightarrow\sigma^{*}\ C_{121}\text{—}O_{122}$	21.86	21.9
$\sigma\ C_{115}\text{—C116}\rightarrow\ \sigma^{*}\ C_{116}\text{—}O_{117}$	4.21	4.21
$C_{115}\text{—}C_{27}\rightarrow\ \pi^{*}\ C_{110}\text{—}C_{114}$	17.30	19.04
$\pi\ C_{115}\text{—}C_{27}\rightarrow\ \pi^{*}\ C_{111}\text{—}C_{117}$	17.75	19.52
$\pi\ C_{115}\text{—}C_{27}\rightarrow\ \pi^{*}\ C_{121}\text{—}C_{126}$	13.67	14.22

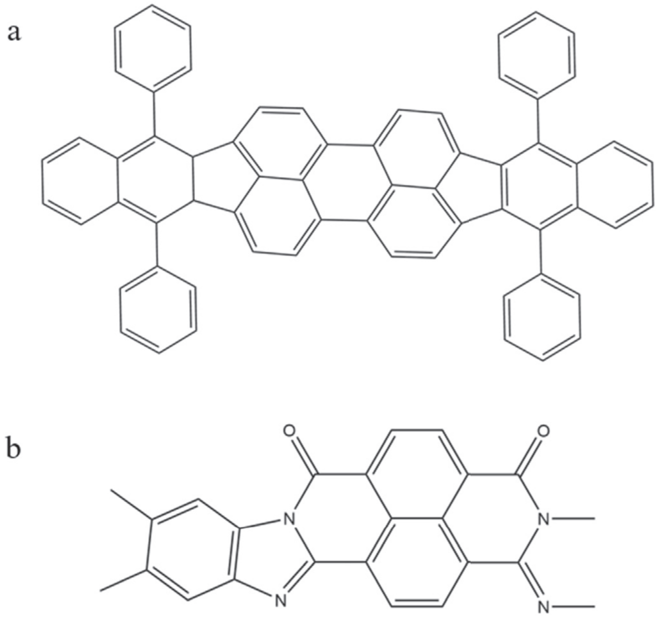

Fig. 1. D-A system structure with (a) DBP as an acceptor and (b) BBL as a donor.

3. Results and discussion

After the geometric optimization of the D-A system, the characteristics of the electron ground state were investigated. In Fig. 2, the energy density of the states is shown for the types of the donor, the acceptor and the D-A system. As it can be seen, the energy gap of A, D and the D-A system is 2.77, 2.35 and 2.03 eV respectively, suggesting that all these components are semi-conductors. Due to this electronic property, A and D can serve as reverse functions when used with strong acceptors and donors. Each of these alone has an energy gap of higher than 2.3 eV. After D-A system construction, the energy gap is decreased to about 0.3 eV. Gap minimization in the electron energy means that the electron transmission from hybrid to non-hybrid orbitals in an excited state is done with less energy. This charge transfer is investigated through the excited state calculations. As it is evident in Fig. 2, the HOMO orbital is located

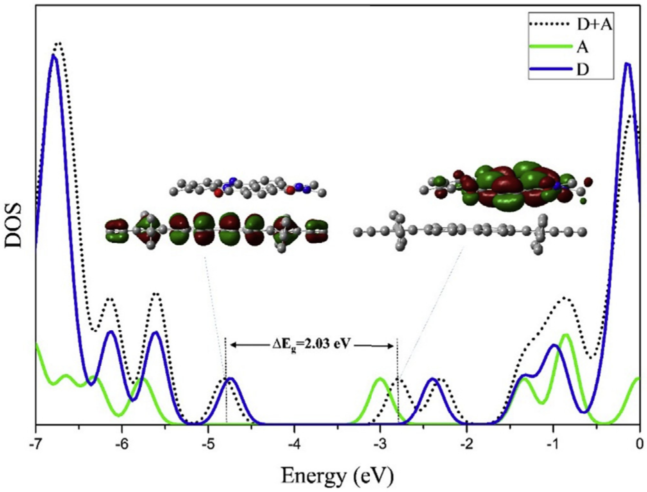

Fig. 2. The images of the HOMO and LUMO orbitals of the D-A system and the DOS graph of A, D and the D-A system.