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A Theoretical Design of a New Organic Dye Containing Coronene for Dye-Sensitized Solar Cells

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ABSTRACT

In search of novel high-performance materials for use in dye-sensitized solar cells (DSSCs), we used density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations to study the geometry, electronic, and optical properties, for organic molecules. The enhancement of organic dye was done by the terminal addition with organic molecule in order to improve their electronic properties and optical absorption. The absorption is became higher than that of the original dye where the rising absorption from 1050 to 1350 approximately. Also, we found that the B3LYP functional with the 6-31G basis set gave highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels. The energy gap decreased after addition from 2.73 to 2.52 eV.

1. Introduction

The current global challenge is to meet the increasing energy consumption with minimum disturbance to the environment [1]. The optimal way to create a modern society powered by electricity it conversion of solar light into electric energy by using solar energy. Therefore, an excellent candidate for a future environmentally friendly energy source there are many technologies have been evolved in relative to solar cells, such the organic solar cells, thin-film solar cells, and dye-sensitized solar cells [2, 3]. A approach for lowering the manufacturing costs of solar cells is to use organic materials and organic solar cells has been developed for more than 30 years [4, 5].

Dye-sensitized solar cells (DSSCs) have been extensively investigated due to their comparable efficiency, simple fabrication process and cost-effectiveness since its invention by O'Regan and Grätzel in 1991 [6], O'Regan developed these dye-sensitized solar cells, the dye is responsible for light-harvesting, charge separation at dye/semiconductor interface, and dye regeneration, etc.,. Typically, a DSSC consisted from of a dye-sensitized TiO_2 nanoparticles, electrolyte and Pt counter electrode, as sandwiched between two fluorine-doped tin oxide (FTO) glass substrate [7, 8]. One of the key materials for DSSC is the TiO_2 that serves the role of dye absorption and electron transport [9]. Given the abundance and variety of dyes, a thorough understanding of their electronic structure and its energy levels are necessary to determine the potential of light harvesting and sensitizing abilities in order to perform in DSSCs [1]. To improve the power conversion efficiency (PCE) of DSSCs, substantial efforts have been devoted to design and synthesis of high effective dyes through reducing molecular energy gap and enhancing optical absorption. So, one needs to optimize the intrinsic properties of donor materials such as highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) and the energy band gap [10, 11].

Particularly, even a minor modification of donor moiety may also lead to prominent changes in cell performance. Thus, it is essential to choose appropriate donor with matched energy levels, strong light absorption, and easy charge separation [7]. The coronene is a single layer of graphite and the smallest fragment of graphene, and consists of sp^2 hybridized carbon atoms [12, 13]. Nanographenes have a great interest owing to their electronic properties touted as the fundamental basis for the next generation of electronic, and photonic devices [14-16].

Computational calculations play a significant role in designing new sensitizers, which provide a profound understanding of the correlation between the structure and properties of the dyes [17].

In this present work, we study the geometry, electronic and optical properties for dye and chemical doping to enhancement these dyes using density functional theory (DFT) and time-dependent DFT (TD-DFT), and to improve the performance of organic solar cells properties. The reason for selecting this dye is that it has been extensively studied experimentally and hence its opto-electronic properties are well described. Furthermore, the donor and acceptor moieties have been considered as building blocks of numerous other dyes for DSSCs. So, our results will be helpful in providing a general understanding of the opto-electronic properties of dyes for DSSCs [18].

2. Experimental Methods

2.1 Computational Methodology

In this article, the geometry optimization of the molecules was performed by using density functional theory (DFT) and time dependent density functional theory (TD-DFT) calculations, as implemented in the Gaussian 09 software [19]. The ground-state geometries of investigated dyes were optimized using B3LYP functional, coupled with the 6-31G basis set [20, 21]. Based on the optimized geometries, HOMO and LUMO energies, energy gap ($E_{gap} = E_{LUMO} - E_{HOMO}$), the total energy E_{total}, the open-circuit voltage $V_{OC} = E_{LUMO}^{Dye} - E_{LUMO}^{TiO2}$ [22], the maximum absorption wavelength λ_{max}, the oscillator strengths (OS) and the UV-Vis spectra were obtained by the associated Gaussview program [23].

3. Results and Discussion

3.1 Geometrical Structure Properties

The geometrical optimization of investigated dye of virtual name (MH) before and after the coronene (C) addition (Fig. 1) was obtained using DFT with B3LYP functional and 6-31G basis set, as shown in Fig. 2.

3.2 Electronic and Optical Properties

The HOMO, LUMO and E_g of the dyes can be obtained by DFT calculations. Fig. 3 shows the distribution of the HOMO and LUMO. The energy gap before and after addition takes the values 2.73 and 2.52 eV, respectively, these values of energy gap for a molecular system provides an indication of its possibility for use as DSSCs. The results indicate that the energy gap becomes smaller of dye MH-C after by adding (C) in the left side because

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of decreasing of the LUMO and increasing HOMO. When the total energy increase as well, this parameter would be of great importance of estimation of stability the structures. The photovoltaic effect is consisted from these steps: first, the photons are absorbed via the material. Second, the excitant delivered from this absorption should be separated, third, the electrodes collect the resulting charge. The electron injection from the excited dye molecule to the conduction band of TiO_2 is more efficient if the LUMO level is higher than the conduction band edge of TiO_2. LUMO must be above the conduction band of TiO_2. The V_{OC} of the dyes with TiO_2 can be estimated in the order of MH (2.20 eV) > MH-C (2.07 eV), the results are summarized in Table 1.

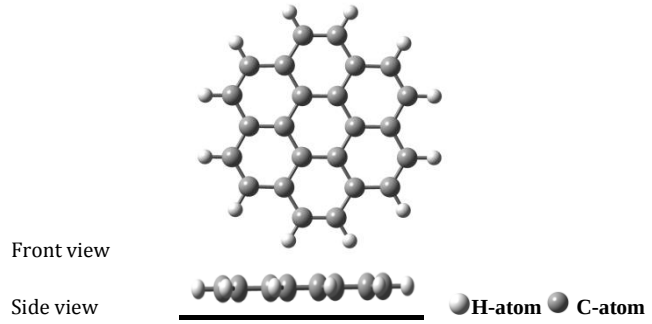

Fig. 1 The addition (C) that use with dye (MH)

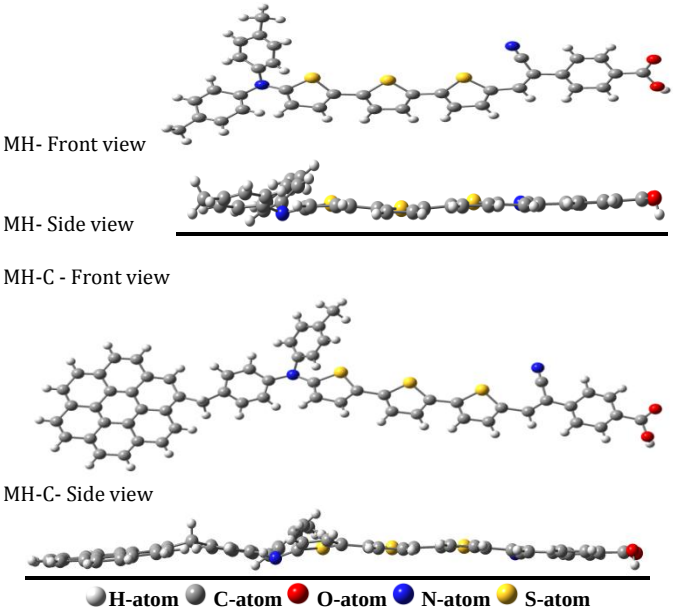

Fig. 2 Geometrical optimization before (top) and after (down) addition of investigation dye at B3LYP functional/6-31G basis set

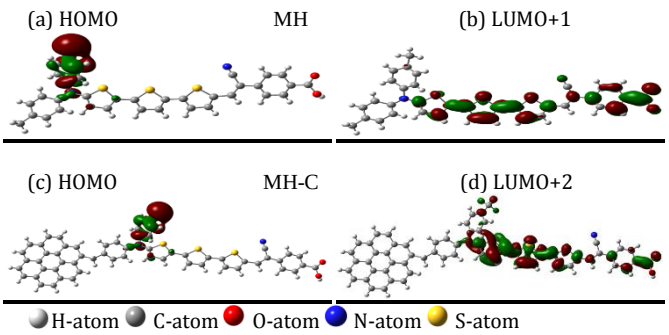

Fig. 3 The localization of HOMO and LUMO before (left) and after (right) improvement of dye

Table 1 Electronic properties parameters (HOMO, LUMO, E_g, E_{total}, and V_{OC}) obtained by B3LYP/6-31G for dyes under study

Dye	H-n* (eV)	L+n* (eV)	E_g (eV)	E_{total} (eV)	V_{OC} (eV)
MH	-4.53	-1.80	2.73	-76903.99	2.20
MH-C	-4.45	-1.93	2.52	-101808.25	2.07

H-n (n = 0,1,2,…); L+n (n = 0,1,2,…); n = 0 , refers to basic HOMO and LUMO

By using the TD-DFT and the B3LYP/6-31G, we calculated the transition states of electron, maximum absorption wavelength λ_{max} and oscillator strengths (OS). These parameters are shown in Table 2. The HOMO part before and after adding has no substantial impact in the orbitals spatial. Whereas the electronic transition changed from LUMO+1 to LUMO+2. The addition of (C) gives the original dye some states of energy as can be shown in Fig. 3(d) since it has high charge mobility. The energy band structures are diagrammed in Fig. 4. From Fig. 5 it is easy to observe that the spectra range from 380 to 1400 (nm) approximately and has little red-shifted with possessing absorption from 1050 to 1350 nm approximately and the value of λ_{max} extends from 498 nm for before addition and 573 nm for after addition. Oscillator strength expresses the strength of the transition for the excited states. The higher the oscillator strength, the higher the possibility of the molecule as a sensitizer. The OS of the dyes in the order of MH (0.0257 eV) < MH-C (0.0303 eV) and this reveals the high light harvesting efficiency.

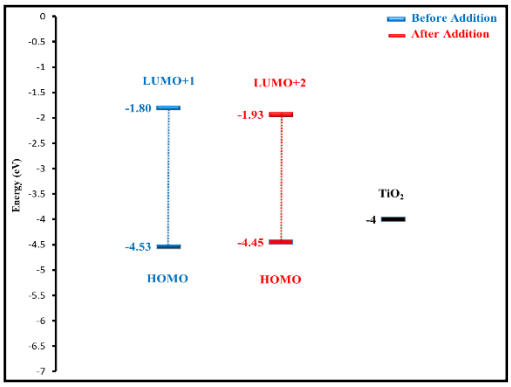

Fig. 4 HOMO and LUMO of dyes and TiO_2 energy levels (blue-plot before addition, red-plot after addition)

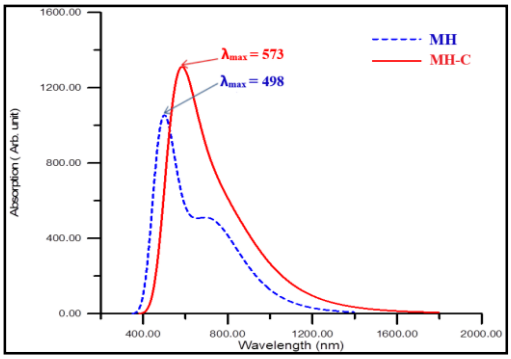

Fig. 5 The absorption spectra of dye before (blue line) and after (red line) addition

Table 2 Data absorption spectra obtained by TD-DFT method with B3LYP/6-31G for dyes under study

Dye	Electronic Transition	λ_{max} (nm)	OS (eV)
MH	HOMO->LUMO+1 (92%)	498	0.0257
MH-C	HOMO->LUMO+2 (80%)	573	0.0303

4. Conclusion

Organic molecules (MH and MH-C) have been investigated using DFT and TD-DFT methods at the B3LYP/6-31G basis set to compute their optimized geometry, electronic, and optical properties. By using DFT method HOMO-LUMO distribution, the energy gap, the total energy and the open-circuit voltage. The energy gap decreases after addition from 2.73 to 2.52 eV. The calculated values of V_{OC}/TiO_2 of our dyes are sufficient for electron injection process from the excited molecule to the conduction band of TiO_2. Therefore, all the studied molecules can be used as sensitizers. Using TD-DFT method, the addition (C) was very suitable for rising the absorption from 1050 to 1350 nm when compared with original dye (MH). The results of this work significantly inspire further molecular engineering of organic sensitizers, enhancing the practical application of dye-sensitized solar cells.

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