Enhancement the electronic and optical properties for the dye Disperse Orange 13 and using in the solar cell device

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Abstract: Disperse Orange 13 (DO13) is from the Azo dye group, its double azo class. It has a good photo-thermal stability dissolvability and easy preparation so that can be used in optoelectronic applications. In this study, three new dye structures group were designed by adding molecular of thiadiazol, thiophene and oxadiazole to DO13 molecular structure, respectively, to enhance the optical and electronic properties of disperse orange 13 azo dye. This study involves investigation and calculation of the optical and electronic properties. energy band gaps, absorption spectrum as a function to wavelengths, frontier orbital (the highest and lowest molecular; the first is occupied and the second is unoccupied orbital), maximum energy, Fermi energy levels, work functions are studied based on the first concepts of the density functional theory (DFT) calculations. The study results show an enhancement on optical and electronic properties of DO13 dye. Where the \( \lambda \) maximum values ranged from 454.670 to 496.760 nm, these values are within the visible light region, the absorption increasing from 0.693 for DO13 to 1.288 for DO13-3thiophene. According to all characteristics shown in the study, the new dyes group may be considered a promise material for solar cell applications.

Keywords: DFT; DO13; energy gap, Gaussian, solar cell

1. Introduction

Materials are assumed an inexorably significant in the technological evolution of photovoltaic solar cell (PVs) and optoelectronic applications[1]. They enhance the quality of optoelectronic devices such as organic light-emitting diodes (OLEDs) and organic solar cells are required to find a new material have a good electro-optical property. That matching with this applications requirement, or improve existed materials properties by using one of the materials preparation method such as dye doping polymers to enhance the polymer properties, by molecular doping process[1–3]. The real challenge for
the researcher is to find or design synthesis of new absorber/donor materials to improve the device performance and lifetime of organic PV solar cells. Therefore, organic solar cells have become a sore topic in recent years. Such new interest is motivating because of their advantage in optoelectronic applications and PV solar cell in special[4]. To begin with, it has been shown that transferring the electron between an excited polymer and C_{60} is so fast and high, this process called the quantum efficiency, which makes it a promising for change carrier separation in solar cell applications. Furthermore, the improvement of efficient organic displays based on OLEDs shows us that what is possible technologies developed for OLED can be used for solar cells applications. In addition, they are helpful to process furthermore, can be utilized to create cheap devices [5].

Macromolecules dyes with π-electrons conjugated which depends on other bonds alteration that can be single or double. The π-electrons conjugation basic principles belong to that π electrons are more flexible regarding to σ electrons. Thus, its moving can be repeatedly done from a site to another when the π electrons moved [6]. These π electrons allow to the light absorption process in another mean (solar cells), and outflow (OLEDs) in these conjugated natural materials. Molecular π-π* orbitals resemble correspondingly to the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO)[6–8].

Disperse Orange 13 (DO13), was chose for this study from the Azo dye group, its double azo class. It has a good photo-thermal stability dissolvability and easy preparation so that can be used in optoelectronic applications, DO13 molecular structure is shown in Fig. 1 [9]. Three new dye structures group were designed by adding molecular of thiadiazol, thiophenes, and oxadiazole to DO13 molecular structure, respectively, to enhance disperse of orange 13 electro-optical properties. First group (thiadiazol group): are designed by adding one, two, and three thiadiazol molecular to DO13 molecular structure, respectively.

Second and third dye group are like thiadiazol group with replacement of the thiadiazol molecular by thiophenes molecular for 2nd dye group (thiophenes group), and oxadiazole molecular for third dye group (oxadiazole group), respectively. The molecular structures of the new three groups of dyes are shown in Figure1.
Figure 1: Geometric optimization of pure DO13 dye structures, and all three dyes groups in study, where the bond length in $\text{Å}$ unit.

Derivatives of thiadiazole are increasingly applied actively in many applications in the arenas of PV applications since they exhibit alluring optical and electronic properties. In addition, many electrons with similar structures have been had by these derivatives to triazoles, oxadiazole, and thiophenes [10].

Several researchers presented the thiadiazols and derivatives for use in solar cell applications. In 2013 Wenjie Fan and Wei-qiao Deng presented theoretical studies use the thiadiazol derivatives as the $\pi$-spacer for the applications in dye-sensitized solar cells (DSSCs) [11].

At the same year, (Higashihara et al., 2013) synthesis new thiadiazol-containing $\pi$ conjugated polymer by the style of reactions that can be described as coupling of 2,5-bis(5'-bromo-3',4'-dihexylthien-2'-yl)-1,3,4,-thiadiazole with various distantly compounds as acceptor and donor monomer unit[12].

In 2014, Wangqiao Chen and etc. study how the thiadiazol group will affect the device performance in bulk heterojunction organic photovoltaics with poly(3hexylthiophene) as donor active media[13].

In 2016 Cheng Chen etc. have designed and synthesized a novel molecular material, which the core unit, benzodithiophene (BDT), was functionalized by thiophene and thiadiazol derivatives to generate extended $\pi$-conjugation. The study shows high gap mobility and high conductivity and the fabric contains a great candidate for application both in perovskite sun based cells (PSCs) as dopant-free gap transport fabric (HTM) and in OSCs as benefactor fabric [14].

After one year Liping Zhu and etc. designed and synthesized a novel small-molecule, which is based on thiadiazol, used as an electron extraction material for perovskite solar cells (PSCs)[15].

In the same year, Alrikabi presented a theoretical survey about the properties that are electronic of graphene nanoflakes where thiadiazols has extended till nine units of the molecule the structures.
Outcomes make clear that enhancing the electronic principles are led by increasing the monomeric units. [16].

And after one-year Alaa M. Khudhair and etc. study theoretically the optoelectronic properties of quarter [1,3,4] thiadiazol and pentathiophene. The donor-acceptor effect group substituents on optical and electronic properties, the study used the (COH, and CP) as substituents for donor group, and (Br, OH, Cl, F, and CN) as a acceptor group substituents. The result of study shows a decrease in the energy band gap. Further, the compounds have major assimilation groups for the sun oriented range, that cruel a great execution for the sun powered cells and photovoltaic gadgets and applications [17].

In this work three new dye structures group were design by additive molecular of thiadiazol, thiophenes and oxadiazole to DO13 molecular structure, respectively, to enhance disperse orange 13 electro-optical properties. The study involves optical and electronic properties, energy band gaps, absorption spectrum as a function to wavelengths, frontier orbital, maximum energy, Fermi energy levels, the functions of work are studied based on the first concepts of the density functional theory (DFT) calculations.

The results obtained from this study showed an enhanced in optical and electronic properties, the oscillator strength reached to 2.900 and 1.288 at wavelength 486.120 nm after additive 3 thiophenemolecular to DO13 dye, while its value was 3.114 for $E_g$ and 0.693 for oscillator strength before the additive. From the result of all characteristics in above, the new dyes group may consider promise materials for solar cell applications.

### 2. Computational detail

All calculations were investigated with Gaussian 09w package [18,19]. The ground state geometries of all studied molecules were optimized with density functional theory (DFT) [20], the functional B3LYP with the 6-31G(d) basis set, the optical properties were also computed with time-dependent (TD-DFT), functional B3LYP[21] with 6-31G(d) basis set [22,23]. We chose the 6-31G(d) basis set as a compromise among the excellence of the theoretical method, and the high computational rate associated with the number of sizes to the problem for all molecules, and because it is well known for its performing appropriately for it in related with optimizing geometry for shells that are closed which in turn can be described as organic compounds [24]. In addition, it is an adequate of describing the collection of systems that are electronic which has a wide range of electrons in molecules that essential through the use of certain sets of bases to have a complete understanding. The electronic properties (total energy ($E_t$), HOMO energies, LUMO energies, HOMO-LUMO gap ($E_g$), and Fermi level energy) were calculated by DFT B3LYP/6-31 (d) basis set, (see table 1). The optical properties (the maximum wavelength, optical energy, and electronic transition) of the systems that are molecular are viewed through the use of TDDFT, 6-31 (d) basis set.

**Table 1**: Total energy ($E_t$ (eV)) Fermi level energy ($E_F$ (eV)) and work function ($\Phi$ (eV)) data, DO13-thiophene structures, calculated for pure DO13 molecules, DO13-oxadiazole, structures and DO13-thiadiazol structures.
3. Results and discussions

3.1. Optimization geometric

All the dyes depend on Disperse Orange 13 (DO13), the optimization geometric of these molecules have been calculated via the DFT B3LYP/6-31G (d) basis set, Fig. 1,2,3, and 4 Illustrations the optimization geometric for all dyes under study. In table 2, we show the lengths that are bond and dihedral points for all the dyes, according to that, Table 2 illustrated that all structures (DO13, DO13-1 thiophene, DO13-2 thiophene, DO13-3 thiophene, DO13-1 thadiazol, DO13-2 thadiazol, DO13-3 thadiazol, DO13-1 oxadiazole, DO13-2 oxadiazole, and DO3 oxadiazole) take the same of values for the bond lengths with different very little. Furthermore, for all the dyes, the dihedral angles also take the same values equal nearly 180°. These results show that all dyes have a configuration of planar; these allude that the including of the azole bunches don't alter within the structures arrangement of all the colors beneath think about (see Fig. 2) and table 2.

|      | Bond Length (Å) | Dihedral Angle (°) |
|------|-----------------|--------------------|
| DO13 | -31073.860      | -4.142             |
| DO13-1 thiophene | -46089.308      | -4.141             |
| DO13-2 thiophene | -61104.729      | -4.130             |
| DO13-3 thiophene | -76120.143      | -4.107             |
| DO13-1 thadiazole | -46962.019      | -4.331             |
| DO13-2 thadiazole | -62850.066      | -4.405             |
| DO13-3 thadiazole | -78738.080      | -4.470             |
| DO13-1 oxadiazole | -38173.267      | -4.331             |
| DO13-2 oxadiazole | -45272.330      | -4.412             |
| DO13-3 oxadiazole | -52371.335      | -4.489             |

Figure 2: Geometric optimization of all study structures, where the bond length in (Å) unit.
Table 2: bond length (Å) and dihedral angle (°) results as calculated by using DFT B3LYP/6.31 (d) for all the structures.

| Sample          | d₁  | d₂  | d₃  | d₄  | θ₁   | θ₂   | θ₃   | θ₄   |
|-----------------|-----|-----|-----|-----|------|------|------|------|
| DO13            | 1.470 | 1.470 | 1.470 | 1.470 | 179.99 | 179.99 | 179.99 | 179.99 |
| DO13-1 thiophene| 1.470 | 1.470 | 1.470 | 1.470 | 179.97 | 179.98 | 180.00 | 179.99 |
| DO13-2 thiophene| 1.469 | 1.469 | 1.470 | 1.470 | 179.99 | 179.98 | 179.91 | 179.91 |
| DO13-3 thiophene| 1.470 | 1.470 | 1.470 | 1.470 | 179.94 | 179.90 | 179.96 | 179.94 |
| DO13-1 thiaodiazole| 1.469 | 1.469 | 1.470 | 1.470 | 179.99 | 179.98 | 179.99 | 179.98 |
| DO13-2 thiaodiazole| 1.470 | 1.470 | 1.469 | 1.469 | 179.99 | 179.98 | 179.98 | 179.98 |
| DO13-3 thiaodiazole| 1.469 | 1.469 | 1.469 | 1.469 | 179.93 | 179.97 | 179.80 | 179.77 |
| DO13-1 oxadiazole| 1.470 | 1.470 | 1.470 | 1.470 | 179.90 | 180.00 | 179.99 | 179.99 |
| DO13-2 oxadiazole| 1.470 | 1.470 | 1.470 | 1.470 | 179.94 | 179.93 | 179.93 | 179.94 |
| DO13-3 oxadiazole| 1.470 | 1.469 | 1.470 | 1.470 | 179.98 | 180.00 | 179.93 | 179.92 |

3.2. Electronic properties

Through the B3LYP/6-31G (d) level, the method of DFT has been used to calculate the electronic properties so as to explain the impact of additive the (thiophene, thiaodiazol, and oxadiazole) on the DO13 dye. Firstly, we tested to appoint the highest steady molecule by know each molecule with its energy, which permissible us to estimate their relative constancies. The stable dye which is greatest is forcefully accredited to the vitality lower [25]. We exhibited that the total energy (E_{\text{total}}) of the dye is enlarged in addition to the (thiophene, thiaodiazol, and oxadiazole) (see Table 1) and (Fig 2), which has great an understanding with the past same recorded considers, this increment made the dye more steady and lower receptive.

Understanding the electronic properties needs to calculate the Fermi energy and the function of the work, it’s so significant parameter for this case. Where the $E_{fL}$ is planned through the below mentioned equation:

$$E_{fL} = (E_{\text{HOMO}} + E_{\text{LUMO}})/2 \quad (1)$$

Further, the $\phi$ is done through this equation:

$$\phi = E_{\text{vac}} - E_{fL} \quad (2)$$

Where $\phi$ represents work function, the $E_{\text{vac}}$ is vacuum level (= 0 eV), and $E_{fL}$ is fermi level.
$E_{fl}$ values changed in the range -3.852 eV to -4.277 eV, while the $\phi$ standards changed from 3.852 eV to 4.277 eV (see table 1), those parameter standards have a good agreement reference [26]. Work function represents the energies that are minimum required in order to remove one of the electrons $E_{fl}$ to the $E_{vac}$. Additionally, from these results of the function of the work $\phi$ demarcate the potential obstruction for the electron emanation for all structures.

To know the effect of the (thiophene, thiadiazol, and oxadiazole) on electronic properties of the DO13 dye, we employed the DFT with the B3LYP/6-31G (d) basis set. The calculated total energy and HOMO-LUMO energies of all the dyes under study are shown in table 3 (see fig 3).

**Table 3:** The electronic transition of molecules, $\lambda_{max}$, $\Omega$, Oscillator strength ($f$), and electronic transition assignments as calculated by using TD-DFT B3LYP/6-31G(d) for all structures.

| Sample          | $\lambda_{max}$ (nm) | $E_{opt}$ (eV) | $E_h$ (eV) | $f$    | Electronic transition   |
|-----------------|----------------------|----------------|------------|--------|------------------------|
| DO13            | 454.670              | 2.726          | 0.388      | 0.693  | HOMO->LUMO (98%)       |
| DO13-1 thiophene| 468.640              | 2.645          | 0.391      | 0.986  | HOMO->LUMO (98%)       |
| DO13-2 thiophene| 479.100              | 2.587          | 0.380      | 1.209  | HOMO->LUMO (96%)       |
| DO13-3 thiophene| 486.120              | 2.550          | 0.350      | 1.288  | HOMO->LUMO (90%)       |
| DO13-1 thiadiazole| 474.620             | 2.612          | 0.391      | 0.817  | HOMO->LUMO (98%)       |
| DO13-2 thiadiazole| 486.690              | 2.547          | 0.380      | 0.861  | HOMO->LUMO (97%)       |
| DO13-3 thiadiazole| 495.280              | 2.503          | 0.332      | 0.807  | HOMO->LUMO (78%)       |
| DO13-1 oxadiazole| 473.460              | 2.618          | 0.391      | 0.796  | HOMO->LUMO (98%)       |
| DO13-2 oxadiazole| 486.050              | 2.550          | 0.383      | 0.832  | HOMO->LUMO (96%)       |
| DO13-3 oxadiazole| 496.760              | 2.496          | 0.340      | 0.786  | HOMO->LUMO (83%)       |

**Figure 3:** The Energy band gap with the number of monomeric units of pure DO13 dye structure, and all three dyes groups in study.

By adding the (thiophene, thiadiazol, and oxadiazole), HOMO energies can be improved and LUMO energies that conduct to decreasing the gap of the electronic energy and the electron injection ability also. Taking the range 2.836-3.114 eV is done by the electronic bandgap energy. Further, the energy gap
that is electronic of all dyes can be reduced and labeled as DO13 < DO13-1 thiophene < DO13-1 oxadiazole < DO13-1 thiadiazol < DO13-2 thiophene < DO13-2 oxadiazole < DO13-2 thiadiazol < DO13-3 thiophene < DO13-3 oxadiazole < DO13-3 thiadiazol, table 3. Having those dyes with their band gaps has a semiconductor demeanor according to the gap of the band which taking the values from 2.836 eV to 3.114 eV (see fig 3).

After that, density of state (DOS) is calculated. That comprises the HOMO and LUMO energies and the energy gap for the all the dyes. The DOS is so meaningful to recognize studying properties that are electronic Fig.4 show the DOS, we noticed that DOS for all the dyes get a similar figure of the form and packers of HOMO, LUMO, and band gap with few disparities in determining the value of the HOMO, LUMO, and gap energy.

**Figure 4:** The density of states (DOS) of pure DO13 dye structure, and all three dyes groups in study.
For the greatest heterojunction solar cells, one from an important parameter for the performance known of PV is the open circuit voltage (Voc), which is depended on the differs between the HOMO and LUMO of the studied dyes. The Voc is possible calculate by using the following equation:

\[ V_{oc} = |E_{HOMO(Donor)}| - |E_{LUMO(Acceptor)}| - 0.3 \]  

(1)

The Voc for all the dyes structures considered are appeared within the Table 4. There are values takes the values from 2.836 to 3.114 eV. These values are exceptionally satisfactory for a plausible the electric move and dynamic electron infusion. At that point, all the dyes beneath study about have utilized as sensitizers due to strategy the electron infusion that asking from the left level to the conduction band is likely within the sensitized of solar cells.

Fig. 5 show the supplying maps for the HOMO and LUMO, for all studied molecules the HOMO is restricted to a very tiny space along with the thiophene at last, whereas, the LUMO appear as restricted great space on the center of the thiadiazol molecules as shown in fig 5.
3.3. Optical properties

The solar cell device efficacy depends on the wavelength check among the kept wavelength group related with the vitality band gap of semiconductor and the wide band of the daylight emanation. In these dyes, the transition states of electron have been explored by utilizing the TD-DFT, the B3LYP/6-31G level, the most extreme retention wavelength ($\lambda_{\text{max}}$), optical energies ($\Omega A$) and oscillator strength ($\Omega$), for the major vital properties of the semiconducting materials. Table 4 are appeared these parameters. The vitality of electronic transition of all dyes is increase with including the (thiophene, thia-diazol, and oxadia-zole) on the DO13 color as seen in Table 4.

**Table 4:** Total energy ($E_t$ (eV)) Fermi level energy ($E_{\text{F}}$ (eV)) and work function ($\Phi$ (eV)) data, DO13 thiophene structures, calculated for pure DO13 molecules, DO13-oxadia-zole, structures and DO13- thia-diazol structures.

| Sample        | HOMO   | LUMO   | $E_g$  | $V_{\text{oc}}$ |
|---------------|--------|--------|--------|-----------------|
| DO13          | -5.699 | -2.585 | 3.114  | 2.814           |
| DO13-1 thiophene | -5.659 | -2.623 | 3.036  | 2.736           |
| DO13-2 thiophene | -5.614 | -2.647 | 2.967  | 2.667           |
| DO13-3 thiophene | -5.557 | -2.658 | 2.900  | 2.599           |
| DO13-1 thia-diazole | -5.832 | -2.830 | 3.003  | 2.702           |
| DO13-2 thia-diazole | -5.869 | -2.942 | 2.927  | 2.627           |
| DO13-3 thia-diazole | -5.887 | -3.053 | 2.835  | 2.534           |
| DO13-1 oxadia-zole | -5.836 | -2.827 | 3.009  | 2.227           |
| DO13-2 oxadia-zole | -5.879 | -2.946 | 2.933  | 2.633           |
| DO13-3 oxadia-zole | -5.907 | -3.071 | 2.836  | 2.536           |

These results illustrate that the aggregate of the $\pi$-conjugation facility, the electrons transmittal from HOMO to LUMO, where the molecular $\pi-\pi^*$ orbitals suggested to HOMO and LUMO. The electron transition in these dyes among neighboring orbitals. For these dyes the $\lambda_{\text{max}}$ values take the extend from 454.670 to 496.760 nm, the most reduced esteem for DO13 and most noteworthy for the DO13-3.
oxadiazole but with a less assimilation. The parameters of the optical properties of all dyes appeared in Fig. 6 from this fig. we watched that the $\lambda_{\text{max}}$ for all the dyes are inside the visible light region.

Figure 6: Absorption spectra of the studied structures, which calculated with TD-DFT B3LYP/6-31G (d), where a: for pure DO13 and DO13- thiophene structures, b: for pure DO13 and DO13- oxadiazole structures, and c: for pure DO13 and DO13- thiadiazol structures. For all the examined structures that are displayed an assimilation range harmonizing to HOMO $\rightarrow$ LUMO. From Table 4, we observed that all the dyes under study have close values from ranging from 83% to 98%, moreover DO13-2 thiophene and DO13-3 thiophene have a strong absorption, and DO13 and DO13-3 oxadiazoole have a less absorption. the location of HOMOs and LUMOs are been shown, in addition to, the electron transition included, well-cleared that the vital PAHs for these particles is affluent with the electrons. This characteristic can empower handle exchanging of the charge in these structures and effuse the electronics against all particles.
4. Conclusions

In this paper, three new dyes structures group were design by additive molecular of thiadiazol, thiophenes and oxadiazole to DO13 dye molecular structure, respectively, to enhance disperse orange 13 electro-optical properties. DFT B3LYP/6-31G(d) technique used to investigate the optimization geometric, electronic stuffs, and optical properties. The study results show, All the study dyes structures show more stable and lower reactive regarding to increases in total energy.

Additionally, the work functions are critical parameters within the field of the light outflow for photoelectronic applications, extended from (3.852 - 4.277) eV. Also, by the adding (thiophene, thiadiazol, and oxadiazole), the HOMO and LUMO energies are improve by cause to decreasing the $E_g$. Where it takes the range from 2.836 eV for pure DO13 dye to 3.114 eV for DO13-3 thiadiazol. And according to the $E_g$ values all the study structures has a semiconductor demeanor.

Also, in the study intended the density of state (DOS) which comprises the HOMO and LUMO energies and the energy gap for the all the dyes, the DOS is so meaningful to recognize studying properties that are electronic. That DOS for all the dyes have the same figure of the shape and packer of HOMO, LUMO, and band gap with few disparities to value the HOMO, LUMO, and energy gaps. Moreover, the study calculated the open circuit voltage (Voc), its one from a vital parameter for the execution known of cells that can be described as solar that are depended on the differs between the HOMO and LUMO in studying dyes. The Voc values for all the dyes molecules studied are in the range from 2.836 to 3.114 eV. This value is very passable for a credible the electric transition and active electron injection.

The greatest absorption wavelength ($\lambda_{\text{max}}$), optical energies ($\Omega$A) and oscillator strengths ($f$), for the major vital properties of the semiconducting materials. Those types of parameter investigated in the study and the result shows the energy of transition that is electronic of all dyes is increment in addition to add the (thiophene, thiadiazol, and oxadiazole) on the DO13 dye. Moreover, the $\lambda_{\text{max}}$ receives the value from 454.670 to 496.760 nm; the smallest values for DO13 and largest the DO13-3 oxadiazole but with a less absorption. That mean the $\lambda_{\text{max}}$ for all the dyes are inside the unmistakable light locale. In addition, all the dyes under study have close values from ranging from (83% to 98%), moreover DO13-2 thiophene and DO13-3 thiophene have a strong absorption, and DO13 and DO13-3 oxadiazole have a less absorption. These comes or result about appear the area of HOMOs and LUMOs, besides, the move of hardware included. This characteristic can empower prepare exchanging of the charge in these structures and effuse the hardware against all atoms. Consequently, the hypothetical ponder gives a great depiction of the electronic and optical properties and allow the superior execution for sun-based cells photovoltaic devices.
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