Molecular Engineering of D-π-A Based on 1,3-Dimethoxybenzene π Spacer for Dye-Sensitized Solar Cells

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A NEW organic sensitizer incorporating D35 as a donor unit, 1,3-dimethoxybenzene as a new π- linker that can be anchored to the TiO2 surface, was synthesized and characterized by UV–Vis, NMR and Mass spectroscopy. The photophysical and electrochemical properties as well as photovoltaic performance of this dye have been studied to evaluate the impact of new π- linker on the power conversion efficiency (PCE) based device. The geometrical configuration of the sensitizer was optimized by density functional theory (DFT) calculations to gain a deep insight into the molecular structure and the electronic properties. Photovoltaic measurements of the present sensitizer in a DSSC configuration was found to show $J_{SC} = 4.0 \text{ mA cm}^{-2}$, $V_{OC} = 610 \text{ mV}$, $FF = 0.53$ and $\eta = 1.3\%$ under standard AM 1.5 G illumination.

Keywords: Photosensitizers, Cobalt electrolyte, TD-DFT; DSSC, π- linker

Introduction

The progress of solar energy technologies offers a hopeful solution to address the global energy crisis. In this respect, dye-sensitized solar cells (DSSCs) are one of the most effective alternate solar cell technologies owing to their cost effective and eco-friendly features [1-5]. Typical DSSC devices comprise a semiconductor photoanode (typically TiO2), a dye sensitizer, an electrolyte and a counter electrode [6]. The dye sensitizer is a crucial component for harvesting sun light and power conversion efficiency (PCE) [7]. In the past decade, researchers have focused on developing new and highly efficient sensitizers. Among them metal-free organic sensitizers have a great deal of interest because of the structural diversity, understandable design, facile molecular tuning, high molar extinction coefficients and tunable photophysical properties [8, 9]. High- efficient organic sensitizers frequently feature a donor--bridge-acceptor (D–π–A) motif. The electronic interaction between donor (D) and acceptor (A) promotes efficient intramolecular charge transfer (ICT) that harvest sunlight for photon-to-electron conversion [10-12].

The studies on D–π–A organic dyes reveal that π-spacer has a significant role in facilitating the electron transfer, regulating the HOMO-LUMO energy gap, extending the absorption range of the sensitizers. Common π-spacers such as phenyl, thiophene, and furan ring have been investigated to increase dyes’ light harvesting capacity and hinder the back electron transfer causing higher performance of their DSSC devices [11, 13, 14].

Regards to donors, several electron rich units such as indoline[15], coumarins [16], phenothiazine [17], Dithienylpyrrole [18], triphenylamines [19-21] have been successfully utilized. Among them, triphenylamine (TPA) moiety can suppress the dye aggregation due to its non-planar structure. Therefore, TPA-based organic sensitizers have revealed great potential in the manufacturing of highly efficient DSSCs devices [22, 23]. The cyanoacrylic acid, as the acceptor group, mainly achieves the prerequisite of an electron acceptor as well as providing the carboxylic acid group for binding the dye to the semiconductor surface [24, 25].

The optimization of the sensitizers is generally based on “guess-and-check” method. In this
respect, density functional theory (DFT) and time-
derpendent density functional theory (TD-DFT) calculations can afford an excellent expectation of
the sensitization properties of the sensitizers upon
the variation of their structure [26].

In the meanwhile, much effort is still needed
for the design and synthesis of novel organic
sensitizers with broad and efficient optical
absorption as well as narrow band-gaps for
DSSCs fabrication. Herein, the influence of
introducing 1,3-dimethoxybenzene as a new \( \pi \)-
linker on the optical and electrochemical
properties as well as PCE of D-\( \pi \)-A organic
sensitizer incorporating D35 as an electron donor
unit is systematically investigated. Furthermore,
DFT and TD-DFT calculations were elaborated in
order to understand the major properties related to
the geometry of the dye. The molecular structure
of the new synthesized dye is shown in Fig. 1.

**Experimental**

**DFT Calculations**

The studied dye was optimized to its lowest
energy using DFT [27] as implemented in
Gaussian 09 software package [28]. The level of
the performed calculation was the hydride three-
parameter density functional method (B3LYP)
[29] which contains the gradient exchange
correction function (B3) along with the correlation
functional [30, 31] this level of calculations was
proved to provide energetic and geometrical
parameters better than other methods [29, 32].
cc-pVDZ [33] was used as the bases set for the
calculation of the optimization due to the large
sterc of the molecule [34, 35].

Furthermore, the basis set 6-31+G was
employed for TD-DFT calculation in order to
generate the first 10 excited states and the total
energy of the molecules. 6-31+G is suitable for
molecules that include large number of atoms
(more than 130 atoms) [36]. Visualization of the
data was performed using Chem Craft 1.6 [37] and
GaussView 5.0 [38] software. The total energy of
the optimized dye, the monovalent cation and
monovalent anion were calculated using the
single point calculation on the same optimized
geometry. Electron affinity (EA) was calculated
as the difference between the total energy of the
neutral dye and that of the monovalent anion (by
removing the hydrogen atom in the carboxylic
group). The ionization potential 18 was calculated
as the difference between the total energy of
the neutral dye and that of the monovalent
cation. Excitation binding energy (\( E_{\text{exciton}} \))
was calculated as the difference between the
LUMO and HOMO in both DFT and TD-DFT
calculations [39]. Normalized excitation binding
energy (\( N_{\text{Ex}} \)) was calculated as the excitation
binding energy divided by the energy of band gap,
to be able to get the effect on excitation binding
energy independent to the value of the bandgap
[40]. Light harvesting efficiency (LHE) of the
studied dyes was calculated as [41]:

\[
\text{LHE} = 1 - 10^{-f}
\]

(Gaussian 09, #28)

**Experimental Materials and Synthesis**

**Chemicals and Solvents**

All solvents were of HPLC grade
quality and used without further purification.
Reactions were carried out under a dry nitrogen
atmosphere. All chemicals including 4-bromo-
2,6-dimethoxybenzaldehyde, palladium(II)
acetate, 2-cyanoacetic acid, tri-o-tolyphosphine,
phosphoursoxychloride, 2,2′-bipyridine,
cobalt chloride hexahydrate (CoCl\(_2\).6H\(_2\)O),
nitrosyl tetrafluoroborate  (NOBF\(_4\)),
ammonium hexafluorophosphate (NH\(_4\)PF\(_6\))
and tetrabutylammonium hexafluorophosphate
(TBAPF\(_6\))  were purchased from Sigma-Aldrich,
Acros or Alfa-Aesar. Electrolyte components–
Co(bpy)\(_3\) (PF\(_6\))\(_2\) and Co(bpy)\(_3\) (PF\(_6\)) were
synthesized according to the literature [42].

**Structural, optical and electrochemical characterization**

\(^1\)H and \(^{13}\)C NMR spectroscopy study was conducted on Bruker 500 MHz instruments by
using the residual signals for CDCl\(_3\) at \( \delta = 7.26
\) ppm and 77.0 ppm as internal references for

![Fig. 1. Molecular structure of the synthesized dye](image-url)
1H and 13C, respectively. PerkinElmer Lambda 950 UV/Vis spectrophotometer was used for recording the UV-Vis absorption spectra of the day in solution and adsorbed on TiO2. The emission spectra were obtained using Jasco FP-6500, Japan spectrofluorometer. All electrochemical measurements were performed in a three-electrode system using Potentiostat/Galvanostat (VoltaLab 40 model PGZ 301), employing a carbon electrode (0: 3 mm) as a working electrode, platinum column as a counter electrode, and an Ag/AgCl electrode as the reference electrode. All data were calibrated with respect to the ferrocene/ferrocenium system. The electrochemical measurements of 0.2 mM of the dye was elaborated in 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF6) in dichloromethane solution as the supporting electrolyte. The voltage is reported with respect to the normal hydrogen electrode (NHE) scale. MALDI-TOF/TOF-MS measurements were carried out using a 4800 Plus MALDI-ToF/ToF mass spectrometer (Applied Biosystems/MDS SCIEX, Foster City, CA, USA) equipped with a Nd: YAG pulsed laser (355 nm wavelength of <500 ps pulse and 200 Hz repetition rate). The 4000 Series Explorer software (V 3.5.3, Build 1017, 2007, Foster City, CA, USA) and the data explorer software (V 4.9, Build 115, 2007, Foster City, CA, USA) were used for analysis. Data acquisition was performed in the reflector positive ion mode. Each mass spectrum obtained was an average of 500 laser shots over the whole spot.

**Synthesis of organic dye**

4′-(bis(2′,4′-dibutoxy-[1,1′-biphenyl]-4-yl)amino)-3,5-dimethoxy-[1,1′-biphenyl]-4-carbaldehyde

A 50 mL two neck schlenk flask equipped with a magnetic stir bar was charged with aldehyde (0.15 g, 0.18 mmol), 2-cyanoacrylic acid (Z25) and [1,3-dimethoxybenzene] in dichloromethane solution as the donor (0.15 g, 0.18 mmol), palladium acetate (6 mg, 0.009 mmol), tri-o-dimethoxybenzaldehyde (0.045g, 0.18 mmol), the catalyst (0.08g, 0.55 mmol), and 20 ml degassed toluene/methanol (6:4). The reaction mixture was heated at 90 °C for 4 h. Next, the mixture was cooled down to room temperature and then washed with ethanol. The residue was washed with brine solution, extracted with ethyl acetate and dried over magnesium sulfate anhydrous. After the solvent was removed under vacuum, the product was purified by silica chromatograph using petroluemth: ethylacate: dichloromethane: (9:0.075:4) as the eluent and a yellowish solid product was gained (0.10g, 65 % yield). 1H NMR (400 MHz, CDCl3) δ 10.51 (s, 1H), 8.01 (s, 2H), 7.47 (d, J = 8.7 Hz, 4H), 7.27 (d, J = 4.7 Hz, 2H), 7.24 (d, J = 9.2 Hz, 2H), 7.19 (d, J = 8.3 Hz, 4H), 6.74 (d, J = 9.4 Hz, 3H), 6.60 – 6.50 (m, 4H), 3.99 (q, J = 12.6, Hz, 8H), 2.95 (s, 3H), 2.88 (s, 3H), 1.76 (m, 13H), 1.56 – 1.34 (m, 8H), 0.99 (t, J = 7.4 Hz, 6H), 0.93 (t, J = 5.4 Hz, 6H)ppm. 13C NMR (100 MHz, CDCl3) δ 189.09, 162.68, 162.64, 162.43, 159.78, 157.11, 148.93, 145.51, 133.76, 133.31, 130.95, 130.44, 127.98, 124.28, 123.15, 123.02, 112.78, 108.11, 105.51, 102.40, 100.61, 68.29, 67.94, 56.53, 56.23, 36.61, 31.57, 31.52, 31.34, 19.47, 19.41, 14.00, 13.96 ppm.

(E)-3-(4′-(bis(2′,4′-dibutoxy-[1,1′-biphenyl]-4-yl)amino)-3,5-dimethoxy-[1,1′-biphenyl]-4-yl)-2-cyanoacrylic acid (Z25)

A 50 mL one neck bottle flask equipped with a magnetic stir bar was charged with aldehyde (0.15 g, 0.18 mmol), 2-cyanoacetic acid (45 mg, 0.53 mmol) and 2-3 drops of piperdine were dissolved in 20 ml of chloroform under inert gas. The reaction mixture was refluxed for 4 h. After that the solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was purified by silica chromatograph using dichloromethane: methanol (9:1) as the eluent to obtain a brown solid product (0.11g, 60 % yields). 1H NMR (400 MHz, Acetone) δ 8.36(s, 1 H), 7.62 (dd, J = 11.9, 8.5 Hz, 1H), 7.48 (t, J = 8.5 Hz, 4H), 7.25 (d, J = 8.3 Hz, 1H), 7.20 (d, J = 8.9 Hz, 1H), 7.13 (d, J = 8.0 Hz, 4H),6.92(d, J = 15.2 Hz, 1H), 6.84(d, J = 14.8 Hz, 1H), 6.62 (d, J = 7.6 Hz, 2H), 6.55 (dd, J = 17.5, 8.2 Hz, 2H), 4.00 (s, 3H), 3.93 (q, J = 21.2 Hz, 8H), 1.80 – 1.62 (m, 8H), 1.56 – 1.41 (m, 8H), 0.98 (t, J = 7.3 Hz, 6H), 0.93 – 0.89 (m, 6H)ppm. 13C NMR (101 MHz, Acetone) δ 159.83, 157.04, 145.66, 133.76, 133.31, 130.66, 130.25, 127.82, 127.79, 123.83, 123.55, 122.61, 122.53, 105.83, 100.27, 67.88, 67.44, 55.62, 55.19, 31.15, 19.16, 19.07, 13.32, 13.30 ppm. MS (MALDI-TOF) m/z calculated for C38H27N2O8 : 916.4734; found, 916.4711 (Supporting information).

**Device Fabrication and testing**

Fluorine-doped tin oxide (FTO) glass substrates were cleaned in an ultrasonic bath using a detergent solution, deionized water and ethanol, respectively (each step 30 min long). The conducting glass substrates were pretreated by immersion in a 40 mM aqueous TiCl4 solution at 70 °C for 20 min and then washed with ethanol.
Scheme 1. Synthetic pathways of Z25 sensitizer

and dried with N2. The triple TiO2 layers on the FTO glass were prepared with an active area of 0.16 cm2 by repeatedly screen printing TiO2 paste (Nanoxide T/SP, Solaronix, Switzerland) and drying at 300 °C between deposition steps. After sintering, the thickness of the films was measured with a profilometer and was ~12 μm. Then, the electrodes were immersed in aqueous TiCl4 rinsed as above and finally sintered at 450 °C for 30 min. When the temperature cooled to 80 °C, the electrodes were immersed into the dye bath containing 0.3 mM of Z25 dye along with chenodeoxycholic acid (0.3mM) in CH2Cl2 and kept at room temperature for 6 h. The photoanodes were then washed with ethanol to remove unabsorbed dye. Platinized FTO was purchased and used as a counter electrode. The Co-based electrolytes consist of: 0.22 M Co (bpy)3(PF6)2, 0.1 M LiClO4, and 0.2 M 4-tert-butylpyridine (TBP) in acetonitrile. The working electrode and the Pt counter-electrode were sealed with a 25 μm thick thermoplastic Surlyn (Meltonix 1170-25, Solaronix, Switzerland) under heating at 120 °C for a few seconds. An electrolyte solution was then injected into the cell through the hole presented in the counter electrode, and the cell was sealed with thermoplastic Surlyn and cover glass to avoid leakage of the electrolyte. The fabricated DSSCs based on Z25 dye were tested under AM 1.5 illumination (100 mW cm−2) using a Keithley Model 2400 source meter. The light source was calibrated with a silicon reference cell before use.

**Results and Discussion**

**Synthesis**

The synthetic pathway of Z25 dye is shown in Scheme 1. The 2',4'-dibutoxy-N-(2',4'-dibutoxy-[1,1'-biphenyl]-4-yl)-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-[1,1'-biphenyl]-4-amine donor was prepared according to literature [43]. The precursor aldehyde was synthesized, in good yield (65%), via palladium-catalyzed Suzuki coupling reaction [44] of 4-bromo-2,6-dimethoxybenzaldehyde with the donor boronic ester with 1:1 molar ratio. Afterward, Z25 was synthesized in a yield of 60 % by Knoevenagel condensation of the aldehyde with 2-cyanoacetic acid in refluxing chloroform using drops of piperidine as catalyst.

**Theoretical studies**

The optimized geometry of Z25 dye is presented in Fig. 2 and its energetic properties are listed in Table 1. The calculations revealed that the bond length values of the C=O and the C-O in the carboxylate group are approximately 1.21 Å and 1.35 Å, respectively. The bond angle C-N-C was ~ 120°, which suggests that the dye has a

![Z25](image)

**Fig. 2.** Optimized geometry of Z25 dye and selected bond lengths shown in angstrom.

TABLE 1. Energetic properties of the studied dye: 
\( E_T \) = total energy, \( \Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \) and 
\( \mu = \) the dipole moment, \( EA = \) electron affinity, \( IP = \) ionization potential,
\( E_{\text{excitation}} = \) excitation binding energy, \( N_{\text{Ex}} = \) normalized excitation binding energy.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_T ) (a.u.)</td>
<td>-2959.2864</td>
</tr>
<tr>
<td>( E_{\text{LUMO}} ) (eV)</td>
<td>-2.3315</td>
</tr>
<tr>
<td>( E_{\text{HOMO}} ) (eV)</td>
<td>-5.0320</td>
</tr>
<tr>
<td>( \Delta E ) (eV)</td>
<td>2.7005</td>
</tr>
<tr>
<td>( \mu ) (Deby)</td>
<td>11.6517</td>
</tr>
<tr>
<td>( IP ) (eV)</td>
<td>5.9974</td>
</tr>
<tr>
<td>( EA ) (eV)</td>
<td>15.0397</td>
</tr>
<tr>
<td>( E_{\text{excitation}} ) (eV)</td>
<td>0.2808</td>
</tr>
<tr>
<td>( N_{\text{Ex}} )</td>
<td>0.1040</td>
</tr>
</tbody>
</table>

The value of the energy gap is of good value to allow the transition between the HOMO and the LUMO of the dye. Furthermore, the energy of the LUMO is lower than the energy of the conduction band of the anatase TiO\(_2\).45 which is frequently used as a semiconductor in DSSCs.46

The electronic excitation properties are given in Table 2 and the calculated absorption peaks of the dye are illustrated in Fig. 3. The excitation data shows two main peaks covering long range of wavelengths in the visible region and proving the dye to be good in DSSC. The frontier HOMO and LUMO distributions are given in Fig. 4 indicate that for the HOMO, the orbital distribution is around the orbitals of the N atom and \( \pi \) orbitals of the rings attached to it and for LUMO, the orbital distribution is around the \( \pi^* \) orbitals of the anchoring group and the ring attached to it. This distribution affords a clear pathway for the charge transfer to the anchoring group and illustrates the opportunity of injection of charge carriers to the semiconductor.

**Photophysical and Electrochemical properties**

The UV-vis absorption and emission spectra of Z25 in CH\(_2\)Cl\(_2\) are illustrated in Fig. 5a-b, and the related data are summarized in Table 3. The measured UV-vis spectrum was as expected from the computational TD-DFT and it shows two distinct absorption bands: the earlier band at \( \lambda = 370 \) nm due to the localized aromatic \( \pi-\pi^* \) electronic transitions.

TABLE 2. Electronic excitation properties of Z25 dye, \( f = \) oscillator strength, \( LHE = \) light harvesting efficiency, \( \lambda = \) wavelength.

<table>
<thead>
<tr>
<th>State no.</th>
<th>Main configuration</th>
<th>Coefficient</th>
<th>( f )</th>
<th>( LHE )</th>
<th>( \lambda ) (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>( H \rightarrow L )</td>
<td>0.70450</td>
<td>0.5514</td>
<td>0.7191</td>
<td>512.43</td>
</tr>
<tr>
<td>S3</td>
<td>( H-2 \rightarrow L )</td>
<td>0.66657</td>
<td>0.6330</td>
<td>0.7672</td>
<td>369.08</td>
</tr>
<tr>
<td>S5</td>
<td>( H \rightarrow L+1 )</td>
<td>0.55028</td>
<td>0.6008</td>
<td>0.7493</td>
<td>351.21</td>
</tr>
</tbody>
</table>

Fig. 3. Calculated absorption spectra for Z25 dye.
MOLECULAR ENGINEERING OF D-II-A BASED ON 1,3-DIMETHOXYBENZENE II ...

Fig. 4. HOMO and LUMO electronic distribution for Z25 dye

Fig. 5. a) Absorption spectra, b) Emission spectra, c) UV-Vis and Emission spectra of Z25 dye in CH₂Cl₂, and d) UV-visible absorption spectra of Z25 dye adsorbed on TiO₂.

transitions of the main conjugated skeleton, and the second band at 420 nm is related to the ICT transitions from the donor to the acceptor of the chromophore. In CH$_2$Cl$_2$, the dye shows intense red fluorescence with $\lambda_{\text{em}}^{\text{max}} = 573$ nm due to the charge transfer to the electron accepting groups. The optical band gap energy ($E_{0-0}$) of 25 assessed from the onset of the absorption and emission spectra (Fig. 5c) was 2.41 eV.

Figure 5d illustrates the absorption spectrum of Z25 adsorbed on TiO$_2$ film. Compared to the absorption spectrum in CH$_2$Cl$_2$ solution, the ICT band for Z25 sensitizer is broadened and red-shifted, indicating the formation of J-aggregation of the dye on the TiO$_2$ surface [47]. Figure 6 displays the cyclic voltammogram of Z25 dye and the corresponding data are depicted in Table 1. The dye exhibits two oxidation and reduction peaks.

![Absorption spectrum of Z25 adsorbed on TiO$_2$ film](image)

**Figure 6.** Cyclic voltammograms of Z25 dye measured in CH$_2$Cl$_2$ solutions at room temperature.

![J-V characteristics of the DSSCs devices based on Z25 dye and the Co$^{II/III}$ electrolyte](image)

**Figure 7.** J-V characteristics of the DSSCs devices based on Z25 dye and the Co$^{II/III}$ electrolyte.

### Table 3. Absorption, emission and electrochemical data for the dye measured in CH$_2$Cl$_2$ solution.

<table>
<thead>
<tr>
<th>Dye</th>
<th>$\lambda_{\text{abs, max}}$ (E) [nm(M$^{-1}$ cm$^{-1}$)]</th>
<th>$\lambda_{\text{em, max}}$</th>
<th>$E_{\text{HOMO}}$ $^a$ [V vs NHE]</th>
<th>$E_{\text{HOMO}-\text{LUMO}}$ $^b$ [eV]</th>
<th>$E_{\text{HOMO}}$ $^c$ [V vs NHE]</th>
<th>$E_{\text{LUMO}}$ $^d$ [V vs NHE]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z25</td>
<td>331(18371), 420 (8500)</td>
<td>573</td>
<td>1.00</td>
<td>2.41</td>
<td>0.87</td>
<td>-1.41</td>
</tr>
</tbody>
</table>

*Fig. 6. Cyclic voltammograms of Z25 dye measured in CH$_2$Cl$_2$ solutions at room temperature.*

*Fig. 7. J-V characteristics of the DSSCs devices based on Z25 dye and the Co$^{II/III}$ electrolyte.*

*Table 3. Absorption, emission and electrochemical data for the dye measured in CH$_2$Cl$_2$ solution.*

MOLECULAR ENGINEERING OF D-Π-A BASED ON 1,3-DIMETHOXYBENZENE Π ...

under the experimental conditions illustrated in experimental section. The initial peak around 0.87 V vs. NHE, is related to the HOMO level, while the other peak is due to the redox potential of the HOMO-1 orbital. The oxidation potential of the excited state of Z25 sensitizer is more negative than the conduction band edge of anatase TiO₂ (E_{cb} = −0.5 V vs. NHE) [48], and its ground state oxidation potential is more positive than the Co^{II/III} (+0.56 V vs. NHE) [42] redox shuttle. Therefore, the synthesized dye is capable to act as sensitizer in DSSC devices where the dye can allow the electrons to be transferred from its LUMO into the conduction band of TiO₂ and enable the dye regeneration by electron transfer from cobalt ions in the electrolyte.

a) Calculated from the intersection of the normalized absorption and emission spectra; b) The ground-state oxidation potentials of the dyes were estimated under the following conditions: Pt as counter electrode and glass carbon working electrode. The electrolyte consisted of 0.2 mM dye and 0.05 M [Bu₄N]PF₆ in dichloromethane. The reference Ag/Ag⁺ electrode was calibrated against an internal Fc/Fc⁺ reference (E° (Fc/Fc⁺) = 0.63 V vs. NHE) c) Estimated by subtracting E₀–0 from the oxidation potential [49].

Performance of the sensitizers in DSSCs

The Z25 sensitizer-based DSSC was fabricated along with the cobalt-based electrolyte and its photovoltaic performance was evaluated. Figure 7 demonstrates the current-voltage (J-V) curve of the fabricated DSSC-based Z25 dyes under AM 1.5G illumination. The DSSC fabricated using Z25 dye showed the performance metrics of JSC = 4.0 mA cm⁻², VOC = 610 mV, FF = 0.53 and η = 1.3%.

Conclusion

The designed and synthesized dye was proved to be a good sensitizer in the visible region and it covers a long range of wavelengths with two peaks of high LHE against two different regions of the visible light. This proves that the 1,3-dimethoxybenzene was good as a π-linker that transfer charge effectively between the donor towards the acceptor and the anchoring group which will inject the charges easier to the semiconductor in the solar cell.

Acknowledgments

The Authors acknowledge the financial support from The Science and Technology Development Fund (STDF) provided by the Egyptian Government for chemical and measurements (Grant # 5415 from Nov. 2014 to Feb. 2018).

Conflict of Interest

There is no conflict of interest

Data Availability

The data used to support the findings of this study are in separated file or available from the corresponding author upon request. (The supplementary data contains ¹HNMR, ¹³CNMR and mass spectra of synthesized compound Z25)

References


MOLECULAR ENGINEERING OF D-Π-A BASED ON 1,3-DIMETHOXYBENZENE Π...


40. Sengul O.; Boydas E. B.; Pastore M.; W. Sharmoukh; Ph. C.Gros; S. Catak; A. Monari, Theoretical Chemistry Accounts, 136 (6), 67 (2017).


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الهندسة الجزيئية لمركب صبغي من النوع معطي- باي- مستقبل للالكترونات يعتمد على 1-3 داي ميثوكثي بنزين للإستخدام في خلايا الطاقة الشمسية الصبغية

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تم تحضير مركب عضوي جديد يشتمل على مركب 1,3-dimethoxybenzene كوحدة مانحة، D35 كوحدة مانحة، و D2TiO2.

جيزة مدينة مغلفة ومستقلة عن الأشعة السينية والفقوق بنفسجية، و ترتيب كريستال الجيني، وعلى محوبيلة كيميائية، وكذلك الأداء الصناعي لهذه الصبغة، تعتمد في تأثير الرابطة للظهیرة الجديدة على خصائص الطاقةнная (PCE). وقد وضح تحسين في القياسات الإلكترونية وخصائص الكهرومغناطيسية. وتم الحصول على قياسات كهرومغناطيسية للمركب الجديد عند استخدامه في تكوين الخلايا الصبغية DSSC ملاحظة: 

القياسية AM 1.5 G تحت إضاءة تحت إضاءة 1.3 و FF = 0.53 و VOC = 610 mV و ISC = 4.0 mA cm⁻²