



## Theoretical study on the application of double-donor branched organic dyes in dye-sensitized solar cells



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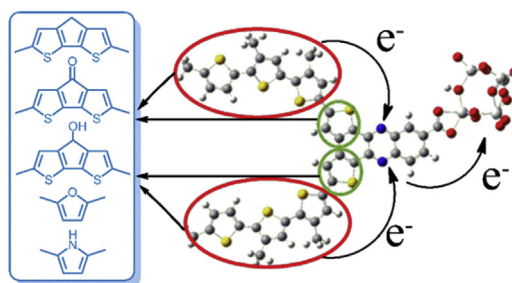
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### HIGHLIGHTS

- A novel organic dye with 2D-A structure was designed and characterized.
- The double-donor branched dye was consisted of two separated light-harvesting paths.
- The double-donor branched dye was beneficial to photocurrent generation.
- The molar extinction coefficient was greatly improved in this novel structure.
- Four promising candidates have been screened out.

### GRAPHICAL ABSTRACT



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### ABSTRACT

A novel organic dye with 2D-A structure has been designed and calculated whereby density functional theory (DFT) and time-dependent density functional theory (TD-DFT) for dye-sensitized solar cells. The double-donor branched dye which was consisted of two separated light-harvesting moieties was beneficial to photocurrent generation. First, we discussed the effects of different donor chains on photoelectric performance in the dye molecule, using the DTP-B8 which was a previously reported structure as the reference. Only to conclude that the suitable length can achieve the satisfactory efficiency. Secondly, to modify and sift potential sensitizers further, three series of dyes (BC-series, CB-series and CC-series) were designed and characterized. The increased molar extinction coefficient and the red-shifted  $\lambda_{\max}$  was attributed to an increasing in electron conjunction. This work presented a new route to design sensitizers that provide two channels for donating more electrons and improve the final efficiency. It is expected to provide some theoretical guidance on designing and synthesizing high efficiency photo-sensitive dye in the future experiments.

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## 1. Introduction

As one of the most affluent renewable energy resources, solar energy has the unique advantages and dramatic potential to be developed and utilized in the near future. Converting solar energy into electricity is an effective way to take full use of solar power.

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Compared with the conventional silicon-based ones [1], the dye-sensitized solar cells (DSSCs), as the third generation organic solar cells, have drawn much attention and attached great importance for its high theoretical photon-to-electron conversion efficiency, abundant reserves of the raw material, friendly to environment and easy to manufacture. Up to now, DSSCs emerged as the new generation organic solar cells have reached an overall conversion efficiency over 13% [2].

For absorbing sunlight and initiating electron transfer reaction, the organic sensitizer has become the most critical components in the DSSCs, determining the efficiency of the device. Moreover, the sensitizers also played a momentous role in influencing many interfacial processes, such as hole injection, charge recombination and a series of photoelectric chemical reaction, all these factors may arouse a significant effect on the power conversion efficiency [3] (PCE).

DSSCs' architectures included D- $\pi$ -A [4–7], D-A- $\pi$ -A [8–10], D-D- $\pi$ -A [11,12], double D- $\pi$ -A [13] and so on. In 2012, Bures et al. have designed and synthesized two series of new D- $\pi$ -A chromophores with double  $\pi$ -linkers [14]. Exploring the  $\pi$ -linker length and chromophore planarity have an effect on the efficiency of intramolecular charge transfer. With increasing  $\pi$ -linker length, the first oxidation potentials did not show significant changes and the first reduction potentials decreased. In contrast to series a, series b possessed an additional triple bond, further planarized the entire  $\pi$ -conjugated system and improved D-A conjugation. These structure-property relationships indicated prospective application in optoelectronic components. However, a new quadrupole D<sub>2</sub>A molecule, which  $\pi$ -bridge unit was not employed and the donors were directly coupled to semiconductor via acceptor, was reported and synthesized including linear (L) and branched (B) configurations by Reynold and his coworkers [15] recently. The main difference between L and B configurations was that the former conjugation was along the donor moieties and the latter conjugation extended all the way through the acceptor. The research demonstrated that the branched organic dyes, compared with linear structure, can increase molar extinction coefficient and provide two avenues to electron moving as well as yield better device performance. In the experiments, DTP-B8 has shown its high molar extinction coefficient and strong absorption performance, with each donors consisting of three thiophene units (as shown in Fig. 1). In this paper, we'll take DTP-B8 as the reference and it exhibit good performance in  $J_{SC}$  (6.01 mA cm<sup>-2</sup>) and  $V_{OC}$  (0.52 V). A series of new D<sub>2</sub>A type dye molecule including B-series, BC-series, CB-series and CC-series were further constructed and designed by selecting structural units of different electronic properties to adjust the performance of sensitizer molecules.

Quantum chemical calculations have become an effective means to evaluate the performance of the DSSCs device and a large number of theoretical work have verified its reliability [16]. In the article, a series of key factors influencing the performance of the cell, including light harvesting efficiency (LHE), electron injection driving force, charge recombination and the shift of conduction band, were simulated and characterized by the methods of the quantum chemistry. Our study revealed how the double-donor sensitizers affect the power conversion efficiency and provided theoretical reference for the future experiment.

## 2. Methods

### 2.1. Theoretical background

As we have known, the power conversion efficiency ( $\eta$ ) which is a momentous parameter to estimate the performance of DSSCs could be expressed by the short-circuit current density ( $J_{SC}$ ), the

open circuit photovoltage ( $V_{OC}$ ) and the fill factor ( $FF$ ), as the following equation [13]:

$$\eta = \frac{J_{SC} V_{OC} FF}{P_{in}} \quad (1)$$

Where  $P_{in}$  is the total solar power incident on the cell. According to Eq. (1), the effective means to enhance  $\eta$  is to improve  $J_{SC}$  and  $V_{OC}$ .

The short-circuit current of the solar cell ( $J_{SC}$ ) is the current (usually the current density) of the solar cell when the external circuit is short. As for  $J_{SC}$  in DSSCs, it can be theoretically expressed as [17]:

$$J_{SC} = \int_{\lambda} LHT(\lambda) \Phi_{inject} \eta_{collect} d\lambda \quad (2)$$

Where  $LHE(\lambda)$  represents the light harvesting efficiency at a given wavelength and  $\Phi_{inject}$  is the electron injection efficiency,  $\eta_{collect}$  is the charge collection efficiency which can be deemed as a constant only little difference in photoactive molecules for a given DSSC because they have same semiconductor electrode (TiO<sub>2</sub>). Based on Eq. (2), The higher  $J_{SC}$  could be obtained via a larger  $LHE$  which could be measured by Ref. [18]:

$$LHE(\lambda) = 1 - 10^{-f} \quad (3)$$

Where  $f$  is the oscillator strength of the dye molecule, the larger  $f$  means a better light capturing. Besides, the total reorganization energy ( $\lambda_{total}$ ) is another important factor to influence the kinetics of electron injection, it can be determined by Ref. [19]:

$$k = A \exp \left[ \frac{-\lambda_{total}}{4k_B T} \right] \quad (4)$$

Where  $A$  is a prefactor,  $k_B$  is the Boltzmann constant and  $T$  is the temperature.  $\lambda_{total}$  is the total reorganization energies, including hole reorganization energy ( $\lambda_h$ ) and electron reorganization energy ( $\lambda_e$ ), is evaluated as [20]:

$$\lambda_{total} = [E_0^\pm - E_\pm^\pm] + [E_\pm^0 - E_0] \quad (5)$$

Where  $E_0^\pm$  is the energy of the anion/cation calculated under the optimized structure of the neutral molecule and  $E_\pm^\pm$  is the energy of the anion/cation based on the optimized geometries of the neutral and anion/cation structure, respectively;  $E_0$  and  $E_\pm^0$  are the energies of the neutral and anion/cation molecules in their ground state and anion/cation state geometries, respectively.

Besides, another critical parameter related to  $J_{SC}$  is the exciton binding energy ( $EBE$ ), which is weighted by Ref. [21]:

$$E_{flu} = \Delta E_{H-L} - EBE \quad (6)$$

Where  $E_{flu}$  is the emission energy from the first excited state to the ground state.  $\Delta E_{H-L}$  is the orbital energy difference between HOMO and LUMO.  $EBE$  is mainly relevant to the efficiency of photocurrent generated, the lower  $EBE$  exhibits the better efficiency.

The open-circuit voltage of the solar cell is the voltage of the solar cell when the external circuit is open, which corresponding to a zero current and infinitely large external resistance. As for  $V_{OC}$  in DSSCs, it can be theoretically described by Ref. [22]:

$$V_{OC} = \frac{E_{CB} + \Delta CB}{q} + \frac{kT}{q} \ln \left( \frac{n_c}{N_{CB}} \right) - \frac{E_{redox}}{q} \quad (7)$$

Where  $E_{CB}$  is the conduction band edge of the semiconductor

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