

Indole-based organic dyes with different electron donors for dye-sensitized solar cells



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ARTICLE INFO

Article history:

Received 5 August 2015

Received in revised form 24 October 2015

Accepted 27 October 2015

Available online 3 December 2015

Keywords:

Indole

Electron donor

Density function theory

Dye-sensitized solar cells

ABSTRACT

Three novel organic dyes **WY1**, **WY2** and **WY3** with the same π -conjugation linker and acceptor but different donor units were synthesized and characterized to investigate the effects of different electron donor units on their photophysical, electrochemical and photovoltaic properties. Density functional theory calculations were carried out to study the ground state geometry structures and electronic structures of the three dyes. Under standard global AM 1.5 solar condition, the solar cells based on **WY1**, **WY2** and **WY3** show the overall power conversion efficiencies as 2.15%, 3.30% and 2.09%, respectively. All the investigation results reveal that different electron donors in organic dyes could cause significant differences in photovoltaic performances and organic dye **WY2** with *N*-hexylphenothiazine as electron donor could show the best performance among the three dyes.

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1. Introduction

The best way to solve the energy and environment issue is to explore clean and sustainable energy. Based on this, solar energy, which is confirmed as the inexhaustible and non-pollution energy source, has attracted researchers' attention. Dye-sensitized solar cell (DSSC), which possesses great application potential for its characteristics of environmentally friendly and low cost, was first developed by O'Regan and Grätzel [1]. Dye sensitizer as one of the components in DSSC always occupies a crucial position for its special role—capture light energy. At present, DSSC based on porphyrin dye has gained the power conversion efficiency (η) of 13% under standard AM 1.5G sunlight [2]. Besides, DSSCs sensitized with N3, N719 and black dye which are all based on ruthenium have also gained relatively high efficiencies [3]. However, the rare of noble metal Ru, environment issues and the complicated preparation procedure have limited the large-scale use of ruthenium-based and porphyrin based dyes. With these in mind, pure metal-free organic dyes have recently been investigated intensively for their advantages of environmental friendliness, high molar extinction coefficient (ϵ), structural

flexibility, low-cost, simple preparation and purification procedures. Recently, the DSSC, which has the efficiency as 12.5%, based on pure organic dye has been reported by Yao et al. [4]. The most common metal-free organic dyes mainly contain triphenylamine dyes [5–7], fluorene dyes [8–10], coumarin dyes [11–13], phenothiazine dyes [14–16], carbazole dyes [17–19] and indoline dyes [20–22].

To date, most of the dyes are characterized with the structure of donor- π -acceptor (D- π -A) [23,24]. Among them, the donor groups can not only affect the absorption spectra but also adjust the energy levels of the sensitizers. And minor changes in the geometry of the donor structure could result in interesting photophysical, electrochemical and other properties [14]. Therefore, the study of the donor group in the D- π -A system is very critical to balance between photovoltage, driving forces and spectral response. Up to now, there are a certain works based on the investigation of the effects of different donor units on the properties of the dyes. Tamilavan et al. investigated the effects of different donor units (methoxy or hexyloxy substituted triphenylamine and difluorenephenylamine) on the properties of the dyes, and they found that the optical, electrochemical and photovoltaic properties of the dyes could be influenced by the steric effect of the electron donor groups [25]. Similarly, Tian and his co-workers also studied the effects of different donor units (10-phenyl-10H-phenothiazine, 10-phenyl-10H-phenoxazine and

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triphenylamine) on the performances of DSSCs. They discovered that the structure variations of electron donor have some degree of influence not only on charge combination, but also on conduction-band edge [26].

In this paper, considering triphenylamine, phenothiazine and carbazole unit are all arylamine units with strong electron-donating ability but different in the structure compared with each other [27], and there is little systematic study based on the three donor units. Hence, three dyes with different electron donor units (triphenylamine (TPA) in **WY1**, *N*-hexylphenothiazine (C₆-PTZ) in **WY2** and *N*-hexylcarbazole (C₆-CBZ) in **WY3**) but the same π -conjugation linker and acceptor were synthesized and applied in DSSCs to investigate the effects of the different donor units on the performances of the DSSCs. The corresponding molecular structures of the three dyes are shown in Scheme 1.

2. Experimental details

2.1. Materials and characterization

Phenothiazine, carbazole, indole-3-carbaldehyde and 4-bromotriphenylamine were purchased from Astatech. Cyanoacetic acid was purchased from Aldrich. The electrolyte consisted of 0.6 M 1,2-dimethyl-3-propylimidazolium iodide (DMPII), 0.025 M LiI, 0.04 M I₂, 0.05 M guanidium thiocyanate (GuSCN), and 0.28 M 4-tertbutylpyridine (TBP) in dry acetonitrile (CH₃CN) was purchased from Heptachroma. All solvents and other chemicals were purchased commercially, and used as received without further purification.

High resolution mass spectra (HRMS) data were measured with a Waters ESI mass spectrometer. ¹H NMR and ¹³C NMR spectra were measured on Brücker AM 400 NMR instrument. The melting points (Mp) data were obtained on X-4 melting point detector (FUKA, Beijing, China). Absorption spectra were measured with SHIMADZU (model UV1700) UV-vis spectrophotometer. Emission spectra were recorded with Hitachi (model RF-5301) spectrophotometer. Cyclic voltammetry experiments were performed on a CH Instruments 660C electrochemical workstation at a scanning rate of 50 mV/s in CH₃CN (5.0 × 10⁻⁴ M) containing 0.1 M *n*-Bu₄NPF₆ as the supporting electrolyte, platinum as counter and work electrodes and Ag/AgCl as reference electrode.

2.2. Preparation of DSSCs

TiO₂ electrodes were bought from Opvtech. When the TiO₂ electrodes were heated to 80 °C for 30 min, the electrodes were immersed in a dye bath containing 0.5 mM **WY1–3** in ethanol and left 12 h. The films were then rinsed in ethanol to remove excess dyes. In our experiment, open cells were fabricated in air by clamping the different sensitized electrodes with a platinized counter electrode. An electrolyte solution was injected into interlayer between two electrodes.

2.3. Photovoltaic characterization

The irradiation source for the photocurrent action spectrum measurement is a photosource (CHF-XM-500W, Trusttech Co., Ltd., Beijing, China) with a CH Instruments 660C electrochemical workstation (Shanghai CH Instruments Co., China). The incident light intensity was 100 mW cm⁻² calibrated with a standard Si solar cell. The tested solar cells were masked to a working area of 0.25 cm². The action spectra of quantum efficiency (QE) for solar cell were performed by using QEX10 quantum efficiency measurement system. Electrochemical impedance spectroscopy (EIS) data were obtained in the dark under forward bias 0.75 V, scanning from 10⁻¹ to 10⁵ Hz with ac amplitude of 10 mV by using CH Instruments 660 C electrochemical workstation.

2.4. Synthesis

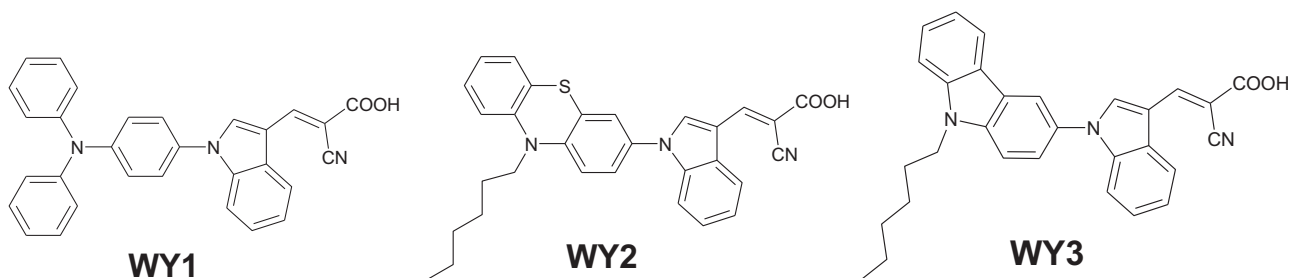
Compound **2a** (**3a**) was synthesized by reacting phenothiazine (carbazole) with bromohexane and in DMF in the presence of NaH at 90 °C [28–31]. Next, compound **2b** (**3b**) was synthesized by reacting compound **2a** (**3a**) with NBS in DMF at low temperature [28,30] (Scheme 2).

Compound 1

A 1,2-dichlorobenzene solution (25 mL) of triphenylamine (0.452 g, 1.40 mmol), indole-3-carbaldehyde (0.261 g, 1.80 mmol), potassium carbonate (0.700 g, 5.07 mmol), activated copper bronze (0.186 g, 2.93 mmol) and 18-crown-6 (0.032 g, 0.12 mmol) were heated under reflux for 48 h. The solvent was removed by decompressing distillation and the residue was purified by column chromatography on silica gel using dichloromethane and petroleum ether (60–90 °C) in the ratio of 2:1 (v/v) as the eluent to give compound **1** as faint yellow solid (0.100 g, yield 18.2%). ¹H NMR (400 MHz, CDCl₃) δ : 10.150 (s, 1H), 7.882 (s, 1H), 7.691–7.675 (d, *J* = 6.4 Hz, 1H), 7.542–7.504 (m, 4H), 7.414–7.334 (m, 10H), 7.203–7.157 (m, 3H). HRMS-ESI (*m/z*): [M–H]⁻ calcd for C₂₇H₂₀N₂O, 387.1576; found, 387.1606.

Compound 2

A 1,2-dichlorobenzene solution (20 mL) of C₆-PTZ (0.505 g, 1.40 mmol), indole-3-carbaldehyde (0.261 g, 1.80 mmol), potassium carbonate (0.700 g, 5.07 mmol), activated copper bronze (0.186 g, 2.92 mmol) and 18-crown-6 (0.032 g, 0.12 mmol) were heated under reflux for 48 h. The solvent was removed by decompressing distillation and the residue was purified by column chromatography on silica gel using dichloromethane and petroleum ether (60–90 °C) in the ratio of 2:1 (v/v) as the eluent to give compound **2** as faint yellow solid (0.125 g, yield 21%). ¹H NMR (400 MHz, CDCl₃) δ : 10.152 (s, 1H), 7.886 (s, 1H), 7.693–7.677 (d, *J* = 6.4 Hz, 1H), 7.545–



Scheme 1. Molecular structures of **WY1–3**.

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