

Comparative study on photovoltaic properties of imidazole-based dyes containing varying electron acceptors in dye-sensitized solar cells



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ABSTRACT

In this paper, a comparative study on the photophysical, electrochemical properties and photovoltaic performances of simple imidazole-based dyes containing varying electron acceptors is done. Two organic dyes containing 4,5-diphenyl-1H-imidazole (DPIM) unit as electron donor and cyanoacetic acid (for **DB-1**) or rhodanine-3-acetic acid (for **DB-2**) as electron acceptor are designed and synthesized. The LUMO and HOMO energy levels of the two dyes can be ensuring positive effect on the process of electron injection and dye regeneration. The overall conversion efficiencies of 1.63% and 0.51% were obtained for DSSCs based on **DB-1** and **DB-2**, respectively. In comparison with **DB-1**, **DB-2** shows the lower J_{SC} , V_{OC} , and efficiency, which is attributed to the lower excited electron injection efficiency and faster charge recombination rate.

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1. Introduction

Dye-sensitized solar cells (DSSCs), developed by Grätzel and coworkers, have attracted considerable attention of many research groups in the past two decades as it offers the possibility of low-cost conversion of the photoenergy [1]. Conventional DSSCs typically contain four components: a mesoporous semiconductor metal oxide film; a sensitizer; an electrolyte/hole transporter; and a counter electrode [2]. In these components, the sensitizer is a crucial element, exerting significant influence on the power conversion efficiency as well as the stability of the cells.

The ruthenium dyes produce overall photo-electrical conversion efficiency of higher than 10% due to their broad photoresponse area [3–5]. However, the manufacturing costs and environmental issues of the ruthenium sensitizers limit their large-scale application. More and more efforts have been dedicated to the development of metal-free organic dyes which exhibit not only higher molar extinction coefficients, but also simple preparation and purification procedures at lower cost. A large number of organic dyes containing nitrogenous electron donors such as merocyanine

[6], indoline [7,8], triphenylamine [9,10], carbazole [11,12] and phenothiazine [13,14] have been used with great success in DSSCs.

Imidazole is also nitrogen compound. It can be used in organic dyes as nitrogenous electron donors based on the following advantages: (1) it is relatively easy to introduce additional electron donors at positions 2 and 4, and an electron acceptor at position 5 of imidazole to form conjugated dipolar compounds [15]; (2) charge recombination after electron injection may be retarded because of decreasing positive charge density at the donor by electronic delocalization of the two substituents at positions 4 and 5 of the imidazolyl ring [16]. Generally, metal-free organic dyes possess the evident molecular structure of the electron donor part and the acceptor part bridged by the conjugated chain (D- π -A). In this structure, small variations within these different sections cause significant differences in photovoltaic properties [14,17].

Based on the above, two new organic dyes containing imidazole units as electron donors and different electron acceptors (cyanoacetic acid for **DB-1** and rhodanine-3-acetic acid for **DB-2**) were designed, synthesized and applied in DSSCs. For the purpose of comparison, dye **L0** with diphenylamine (DTA) unit as electron donor was also synthesized. The design motivation for the two new dyes is to evaluate the feasibility of 4,5-diphenyl-1H-imidazole (DPIM) unit as electron donor for constructing efficient D- π -A organic dye and study the effects of different acceptor in the two dyes on the optical, electrochemical properties and

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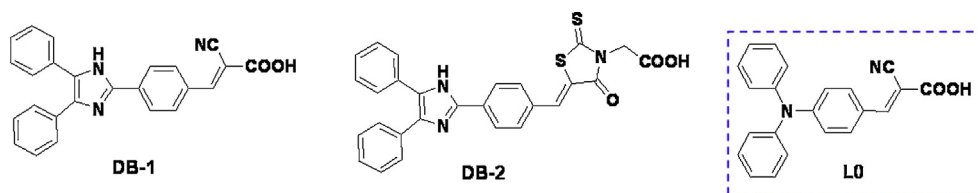


Fig. 1. Chemical structures of dyes **DB-1** and **DB-2** and reference dye **LO**.

photovoltaic performances. The corresponding molecular structures of these dyes were shown in Fig. 1. The photophysical, electrochemical properties and photovoltaic performances of these dyes were investigated by spectral, electrochemical, photovoltaic experiments, and density functional theory calculations.

2. Experimental details

2.1. Materials and characterization

All solvents and other chemicals were reagent grade and used without further purification. Benzil, 1,4-phthalaldehyde, cyanoacetic acid, rhodanine-3-acetic acid and triphenylamine were purchased from Astatech. HRMS data were obtained with a HITACHI-80 instrument. ^1H and ^{13}C NMR spectra were measured on Varian Mercury Plus 400 MHz NMR instrument. M_p data were obtained on X4 melting point detector (FUKA, Beijing, China). INSPECT F Scanning electron microscopy (SEM) (FEI, Netherlands) is used to measure the thickness of the TiO_2 film. Absorption spectra were measured with SHIMADZU (model UV2550) UV–vis spectrophotometer. Cyclic voltammetry experiments were performed on a CH Instruments 660C electrochemical workstation with a scanning rate of 50 mV/s in dimethylformamide (DMF) (5.0×10^{-4} M) containing 0.1 M $n\text{-Bu}_4\text{NPF}_6$ as the supporting electrolyte, platinum as counter and work electrodes and Ag/AgCl as reference electrode.

2.2. Fabrication of DSSCs

TiO_2 colloid was prepared according to the literature [18]. The washed FTO glass substrates were immersed in 40 mM TiCl_4 aq. at 70 °C for 30 min to form a compact layer of TiO_2 , which plays an important role in suppressing the charge recombination of DSSCs at the interface between FTO and electrolyte, then washed with water and ethanol. A thin film of TiO_2 was prepared on the FTO substrate with the compact TiO_2 layer through blade coating with glass rod. After drying the nanocrystalline TiO_2 layer at 80 °C, the TiO_2 thin film with more layers was achieved by repeating the blade coating above process two times. The resulting working electrode was composed of a 15 μm thick transparent TiO_2 nanoparticle layer. Finally TiO_2 electrodes were treated at 450 °C for 30 min. After cooling to room temperature, the electrodes were immersed in

40 mM TiCl_4 aq. at 70 °C for 30 min, and washed with water and ethanol again, then recalcined at 450 °C for 30 min. After the sintering, when the TiO_2 electrodes cooled to 80 °C, the electrodes were immersed in dye baths containing 0.2 mM **DB-1**, **DB-2** and **LO** in ethanol and left overnight. The films were then rinsed in ethanol to remove excess dyes. In our experiment, open cells were fabricated in air by clamping the different dyed electrodes with platinumized counter electrode. The electrolyte used here is composed of 0.6 M 1,2-dimethyl-3-propylimidazolium iodide (DMPII), 0.0653 M LiI, 0.03 M I_2 , 0.28 M 4-*tert*butylpyridine (TBP) and 0.05 M guanidinium thiocyanate (GuSCN) in acetonitrile.

2.3. Photovoltaic characterization

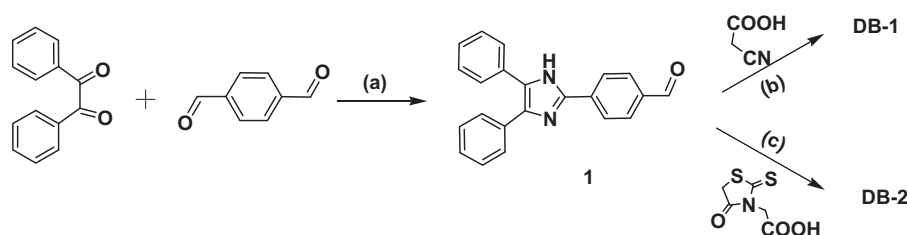
The irradiation source for the photocurrent action spectrum measurement is a photosource (CHF-XM-500W, Trusttech Co. Ltd., Beijing, China) with a CH Instruments 660C electrochemical workstation (Shanghai CH Instruments Co., China). The incident light intensity was 100 mW cm^{-2} calibrated with a standard Si solar cell. The tested solar cells were masked to a working area of 0.16 cm^2 . The action spectra of monochromatic incident photon-to-current conversion efficiency (IPCE) for solar cells were performed by using a commercial setup (QTest Station 2000 IPCE Measurement System, CROWNTECH, USA). Electrochemical impedance spectroscopy (EIS) data were obtained in the dark under forward bias 0.7 V, scanning from 10^{-2} to 10^5 Hz with ac amplitude of 10 mV by using CH Instruments 660C electrochemical workstation.

2.4. Synthesis

Reference dye **LO** was prepared according to the reported literature [19]. The **DB-1** and **DB-2** were synthesized as shown in Scheme 1.

2.4.1. Synthesis of compound 1

A acetic acid (20 mL) solution of benzil (313 mg, 1.49 mmol), 1,4-phthalaldehyde (200 mg, 1.49 mmol) and ammonium acetate (1.8 g, 23.8 mmol) were charged sequentially in a three-necked flask and heated under reflux for 10 h. The reaction mixture was poured into ice-cold water. The resulting precipitates were filtered, washed with water, and dried. Then the residues were purified by silica gel column chromatography with dichloromethane/ethyl acetate (12:1, v:v) as eluent to afford compound **1** as a yellow



Scheme 1. Synthetic routes of dyes **DB-1** and **DB-2**. (a) ammonium acetate, acetic acid, reflux, 10 h; (b) piperidine, acetonitrile, reflux; (c) piperidine, acetonitrile, reflux.

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