



Effects of different solvent baths on the performances of dye-sensitized solar cells: Experimental and theoretical investigation

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ABSTRACT

Combining experimental analyses and computational modeling, we investigated **CD-7**-sensitized solar cells (DSSCs) by THF or DMF bath with aim to understand the effects of different solvent baths on the performances of the corresponding DSSCs. In experiment, the photophysical, photovoltaic and electrochemical impedance properties of the DSSCs based on THF or DMF bath were investigated. The UV–vis spectrum of **CD-7** in THF is red-shifted in comparison with it in DMF, indicating that there are different interactions between **CD-7** and the solvent molecules. The UV–vis spectrum of **CD-7** adsorbed on TiO₂ film suggested that different solvent baths have different effects on the J-aggregation and absorption strength. Monochromatic incident photon-to-electron conversion efficiency (IPCE) and electrochemical impedance analyses showed that different solvent baths have significant influences on the IPCE values and electron lifetimes of the corresponding DSSCs. The analysis results of computational modeling showed that the solvent molecules would affect the energy level of TiO₂, adsorption structure and adsorbed amount of **CD-7** on the TiO₂ film. The above analysis results illuminate a big difference in the performances of DSSCs by THF or DMF bath. The DSSCs based on THF bath obtained the η value 1.53%, which is about twice as much as that of DMF bath.

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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 owing to their high efficiencies and low costs [1]. DSSCs typically contain four components: a mesoporous semiconductor metal oxide film, a dye, an electrolyte/hole transporter, and a counter electrode [2]. Various attempts toward the modification of these different components have been

carried out to improve the overall conversion efficiency of DSSCs. In particular, extensive studies on the development of highly efficient dyes have been carried out as they play a crucial role on the performances of DSSCs. Up to now, DSSCs based on ruthenium dyes and porphyrin dyes have shown very impressive solar to electric power conversion efficiencies. The DSSC based on black dye with donor-acceptor type coadsorbent has reached an overall solar energy conversion efficiency (η) of 11.4% [3], and porphyrin-sensitized solar cell with cobalt (II/III)-based redox electrolyte has obtained a new record efficiency of 13% [4]. On the other hand, the preparation of the dye-sensitized TiO₂ photoelectrode is also important for the higher

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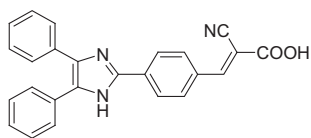


Fig. 1. Chemical structure of dye CD-7.

performances of DSSCs because many photo- and electrochemical reactions, such as photoexcitation of dyes, the electron injection from dyes to TiO_2 , and the reduction of the oxidized form of dyes occur at the dye/ TiO_2 interface.

In the processes of preparing dye-sensitized TiO_2 photoelectrode, the different solvent baths have a crucial effect on the dye-sensitized TiO_2 photoelectrode. To our knowledge, there is a diversified interaction between the dyes and different solvents [5], which could give a different physical and chemical properties to the dyes adsorbed on the TiO_2 surface. Numerous theoretical investigations have examined the adsorption modes of small organic molecules (i.e., formic acid [6–10] and benzoic acid [11,12], isonicotinic acid [13] and bipyridine ligand [14]), small phosphonate group [15], metal-free organic dyes [16–20], and ruthenium-complex [21–25] dyes on TiO_2 surface. The overall view extracted from these works indicates an important role of the dye geometry and adsorption energy on the electrochemical properties and efficiencies of DSSCs. Besides, many theoretical studies have also focused on the characterization of the solvent– TiO_2 interactions (water [6,26–29] and acetonitrile [6,29,30] in both free and dye-sensitized TiO_2). However, a systematic study of the solvent–dye– TiO_2 heterointerface, comparing different solvents, and of the associated structural and electronic distribution changes is still very little.

In this work, a simple organic dye CD-7 (Fig. 1) was designed and synthesized, and it dissolved in DMF or THF were employed to sensitize TiO_2 photoelectrode, and then the photovoltaic and electrochemical impedance performances of the corresponding DSSCs were measured. To gain insight into the effects of different solvent baths on the performances of the corresponding DSSCs, periodic density functional theory (DFT) calculation was used to study the effects of different solvent on the geometry and electronic structure of CD-7 adsorbed on the TiO_2 surface.

2. Experimental section

2.1. Fabrication of DSSCs

TiO_2 colloid was prepared according to the literature [31]. 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 14 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 recalined at 450 °C for 30 min. After the sintering, when the TiO_2 electrodes cooled to 80 °C, the electrodes were immersed in the DMF or THF containing 0.2 mM CD-7 for 12 h, respectively. The films were then rinsed in ethanol to remove excess dye. In our experiment, open cells were fabricated in air by clamping the different dye-sensitized electrode with platinumized counter electrode. The electrolyte used here is composed of 0.6 M 1,2-dimethyl-3-propylimidazolium iodide (DMPII), 6.53×10^{-2} M LiI, 0.03 M I_2 , 0.28 M

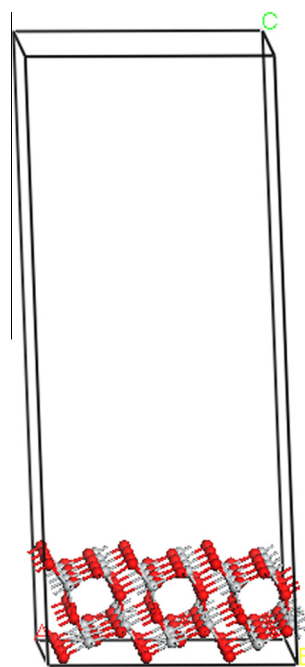
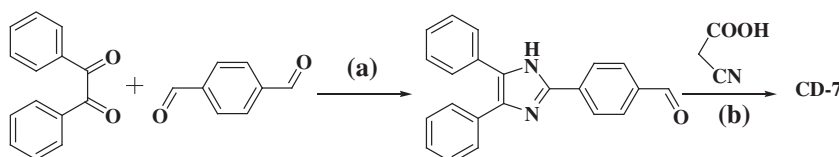


Fig. 2. Geometry-optimized structure of TiO_2 anatase (101) surface.



Scheme 1. Synthetic route of dye CD-7. (a) Ammonium acetate, acetic acid, reflux, 10 h; (b) piperidine, acetonitrile, reflux.

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