



Poly(phenylene cyanovinylenes) carbazole based conjugated polymer as a photosensitizer for dye-sensitized solar cells



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ABSTRACT

A carbazole based new n-type conjugated polymer (**CP**) has been synthesized and employed as a photosensitizer in polymer-sensitized solar cells (PSSCs). The synthesis of **CP** was accomplished by the reaction of appropriate monomer dialdehyde with aromatic dinitriles, under Knoevenagel condensation conditions followed by its characterization by ¹H NMR and FT-IR. The band gap of **CP** measured by cyclic voltammetry (CV), density functional theory (DFT) and diffuse reflectance (DR) UV-vis spectroscopy revealed closely matched values of 2.57, 2.47, and 2.64 eV respectively. Under the illumination of AM1.5G (100 mW cm⁻²), **CP** based PSSCs exhibited power conversion efficiency of 2.08% with a short-circuit current density (*J*_{sc}) of 7.0 mA/cm², an open-circuit voltage (*V*_{oc}) of 534 mV and a fill factor (FF) of 55.85%.

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1. Introduction

As one of the low-cost alternative to conventional inorganic solid state solar cells, dye-sensitized solar cells (PSSCs) have attracted continued interest from the research community [1]. In a typical DSC device, absorption of photon by a highly absorbing photosensitizer that is bounded onto the surface of a metal oxide semiconductor (usually TiO₂) leads to the excitation of its ground-state electron. The resultant excited electron is then injected into the conduction band of TiO₂ and ultimately through an external circuit to a counter electrode. Finally, ground-state structure is regenerated when the electron is taken back into the oxidized dye molecule by a redox shuttle that exists in the electrolytic solution. This cycle is repeated continuously for the generation of electric power from sunlight, without consuming any material. On the other hand, in an organic photovoltaic cell (OPVC), the photo energy conversion of organic solar cells occurs via following four steps: (i) light absorption of donor, leading to exciton formation; (ii) diffusion of the exciton within the active layer to the donor-acceptor interface; (iii) dissociation of exciton from the LUMO (lowest unoccupied molecular orbital) of the donor to LUMO of the acceptor; and (iv) collection of free charge carriers at the electrodes. The role of sensitizer in the photon conversion efficiency (η) is critical and therefore tailoring its design to achieve

higher efficiency is important. In general, the nature of sensitizer is based on metal-based complexes that involve metal-to-ligand charge transfer excited state or metal-free organic dyes. In general, doping of TiO₂ with various dopants is employed to realize efficient photocatalytic activities. Xin et al. have prepared Ti³⁺ doped TiO₂/g-C₃N₄ composites and studied its photocatalytic activity under visible light [2]. Likewise, Ta⁴⁺ self-doped Ta₂O₅ nanorods have also been used in photocatalytic applications [3]. In a recent report, Ta⁴⁺ self-doped quantum dots of Ta₂O₅ and self-doped Ta₂O₅ quantum dots modified with cotton like g-C₃N₄ nanosheets, exhibiting excellent visible light response, have been reported [4]. However, organic dyes are superior to metal-based sensitizers and offer numerous advantages including cost-effectiveness, design versatility, high molar extinction coefficients and relatively good efficiency [5,6]. In recent years, conjugated polymers, with extended π -conjugation, possessing sulfur (polythiophenes) and nitrogen (polypyrroles) as heteroatoms in the polymer main chain are very attractive for a wide range of applications [7,8]. In an earlier report, poly epinephrine and poly dopamine dyes have been synthesized for metal free PSSCs [9], demonstrating larger current density (3.63 mA cm⁻²) and energy conversion efficiency (0.41%). Recently, the deployment of substituted carbazole based dye as a photosensitizer for PSSCs has been reported [10]. The DSC device exhibited higher values of *V*_{oc} (59 mV) and FF (29%) compared to that of reference polymer. Recently, we have reported the synthesis and oxygen evolution reaction (OER) of carbazole-based n-type conjugated polymer [11]. Herein we wish to disclose its performance as

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sensitizer of PSSC. The solar cell assembled using functionalized **CP** as a photoactive layer was characterized by photocurrent–voltage characteristics. Based on the experimental results, the photovoltaic behavior of PSSCs was acceptable, showing power conversion efficiency of 2.08%. This manifested its promise as a polymer photosensitizer for PSSCs.

2. Experimental

2.1. Synthesis of CP

To a solution of mixture of THF (25 mL) and t-BuOH (25 mL) at room temperature was sequentially added diacetonitrile **2** (0.63 g, 1.18 mmol), dialdehyde **6** (0.45 g, 1.18 mmol) and t-BuOK (0.39 g, 2.55 mmol). The mixture was heated for 12 h at 70 °C and then cooled to room temperature upon completion. The reaction mixture was poured over ice cold methanol, acidified with acetic acid (1.5 mL) and precipitates formed were collected by filtration. Re-precipitation of the solid from methanol afforded 0.30 g (65%) of **CP** as dark red amorphous solid. IR (KBr): 3029, 2959, 2929, 2856, 2211, 1599, 1482, 1209, 1032. ¹H NMR (500 MHz, CDCl₃): δ 0.88–0.97 (br. m, 18H), 1.32–1.77 (br. m, 25H), 2.12 (br. s, 1H), 3.84 (br. s, 4H), 4.24 (br. s, 2H), 6.86 (br. s, 2H), 7.06 (br. s, 2H), 7.48 (br. s, 4H), 7.57–7.84 (br. m, 6H), 7.98 (br. s, 2H), 8.45 (br. s, 2H). Anal. Calcd for (C₆₀H₆₉N₃O₂)_n: C 83.39; H 8.05; N 4.86. Found: C 83.02; H 8.28; N 4.51. GPC (PS standard): Number molecular weights (M_n) = 3089, Weight-average (M_w) molecular weights = 6583, PDI = 2.13.

2.2. Fabrication and characterization of PSSCs

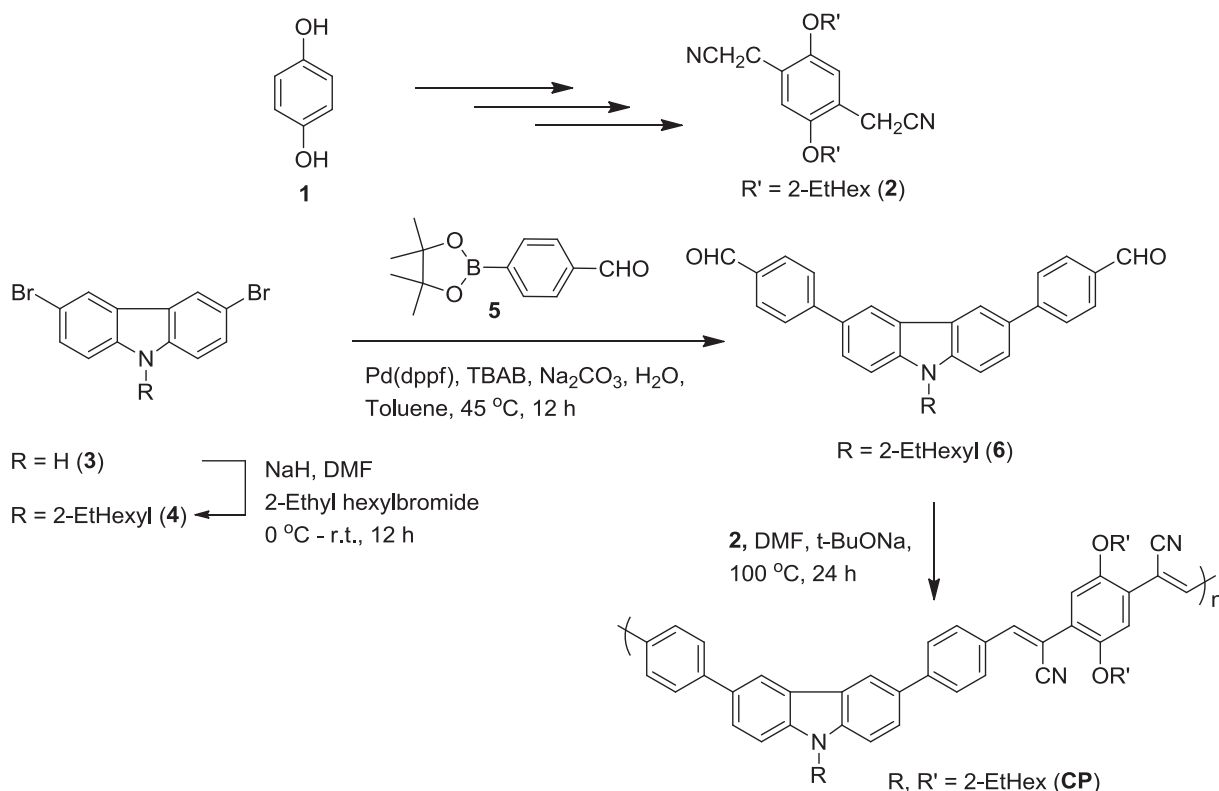
Fabrication and Characterization of PSSCs was achieved according to earlier reported procedures [12].

3. Results and discussions

3.1. Synthesis and characterization of CP

The synthesis of dinitrile monomer **2** was achieved based on literature known procedures [13]. Carbazole **3** was reacted with 2-ethyl hexylbromide to generate N-alkylated carbazole **4** [14]. Likewise, Suzuki-Miyaura coupling reaction between boronic ester **5** [15] and N-alkylated dibromide **4** generated monomer **6** in high yield (80%) [11]. Finally, Knoevenagel condensation reaction between monomers **2** and **6** led to the generation of copolymer **CP** with excellent *E* olefin stereochemistry (Scheme 1). In the FT-IR spectrum, the absence of peaks 2866, 2733 and 1690 cm⁻¹ (aldehyde peaks) and shifting of nitrile absorption around ~40 cm⁻¹ from 2250 cm⁻¹ to ~2211 cm⁻¹ confirmed formation of conjugated cyanovinylene moieties. Similarly, ¹H NMR of **CP** consisted all the relevant diagnostic peaks of carbazole and cyanovinylene (Fig. S-1). In the thermogravimetric analysis (TGA), heating **CP** upto 325 °C with a heating rate of 10 °C min⁻¹ under oxygen atmosphere resulted in no appreciable loss of mass. However, onset decomposition temperatures (T_d) of **CP** was found at 350 °C whereby the polymer started decomposing and further increase in temperature above the T_d led to abrupt loss of weight, hinting decomposition of the backbone of **CP** (Fig. S-2). The UV-vis absorption spectra of **CP** (dilute THF solution), indicated a relatively weak absorption around 330–383 nm and an intense band at around 383–500 nm (Fig. S-3). These bands were attributed to localized π–π* and delocalized π–π* transitions, respectively. The delocalized π–π* transitions were considered due to the internal charge transfer (ICT) interaction caused by the donor and acceptor units of the polymer [16].

Supplementary data associated with this article can be found, in the online version, at <https://doi.org/10.1016/j.matlet.2018.07.122>.



Scheme 1. Synthesis of CP.

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