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New diketopyrrolopyrrole-based organic dyes for highly efficient dye-sensitized solar cells

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ABSTRACT

Three diketopyrrolopyrrole (DPP) dyes (**ICD-3**, **ICD-4** and **ICD-5**) with a D- π -A conjugation were designed and synthesized, where a symmetric phenyl-DPP-phenyl unit was used to connect a substituted diphenylamine and a thienyl acrylic acid, and two *n*-hexyl or 2-ethyl-hexyl chains were introduced on the periphery of the DPP macrocycle. The dyes were characterized by photophysical, electrochemical, and density functional theory calculations. Among the three dyes, the **ICD-5**-based DSC afforded the best photovoltaic performance: a short circuit photocurrent density (J_{sc}) of 16.34 mA/cm², an open circuit voltage (V_{oc}) of 753 mV, and a fill factor (FF) of 0.74, corresponding to an overall conversion efficiency (η) of 9.10% using I^-/I_3^- redox couple-based liquid electrolyte under AM 1.5 conditions. The experimental results demonstrate that the DPP-based sensitizer is a promising option for DSCs, and rational molecular engineering is crucial for constructing highly efficient charge transfer sensitizers.

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1. Introduction

Dye-sensitized solar cells (DSCs) are one of the most promising alternatives to the conventional inorganic semiconductor photovoltaic devices due to their potential low material/fabrication cost and relatively high conversion efficiencies [1]. As one of the key components, the sensitizer is exerting a significant influence on the power conversion and stability in DSCs. With ruthenium complexes [2a–d] and zinc porphyrin dyes [2e–f], high power conversion efficiencies of up to 8–12% have been achieved. On the other hand, metal-free organic dyes, usually with electron donor- π conjugation bridge-electron acceptor (D- π -A) configuration, have been intentionally investigated due to

their molecular tailoring flexibility and raw material abundance, exhibiting comparable conversion efficiencies [3]. In the D- π -A organic dyes, triarylamine and cyanoacrylic acid were widely used as donor and acceptor, respectively, and various π -conjugated bridges were employed to bridge the donor and acceptor units to construct a large number of D- π -A dyes for DSCs. The conjugation bridge is of paramount importance in tuning the molecular energy gap, and the electronic and steric structures, strongly affecting device performances [4].

Diketopyrrolopyrrole (DPP) chromophore has a uniquely planar conjugated bicyclic structure with electron-withdrawing property, and its derivatives are extensively used as high-performance pigments due to its exceptional photochemical, mechanical and thermal stability [5]. Following their successful investigations in a series of optical electronic devices [6], it was first tested as sensitizers for DSCs in 2010 [7a]. So far, a series of

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symmetric and asymmetric DPP dyes have been reported, and the device performances have been greatly improved [7]. In 2012, Han's group introduced a strong electron donor indoline in a symmetric DPP dye, giving efficiency of 7.4% [7d]. Following the report, an asymmetric DPP sensitizer with intense absorption in the red/near-IR region was prepared with an efficiency of 7.7%, and a higher efficiency of 8.6% was achieved by co-sensitization with another spectrally complementary organic sensitizer [7f]. Very recently, the same group furthermore modified the structure of asymmetric DPP sensitizers, giving a high efficiency of 10.1% employing $\text{Co}^{2+}/\text{Co}^{3+}$ redox couple [8]. In our previous report, we found that compact DPP-based dyes **ICD-1** presented broad absorption spectral with efficient charge transfer in the molecule, leading to a power conversion efficiency of 8.61% in DSC with an I^-/I_3^- redox couple-based electrolyte [9]. Therefore, DPP-based sensitizers is a desirable building block for constructing highly efficient sensitizers in DSCs.

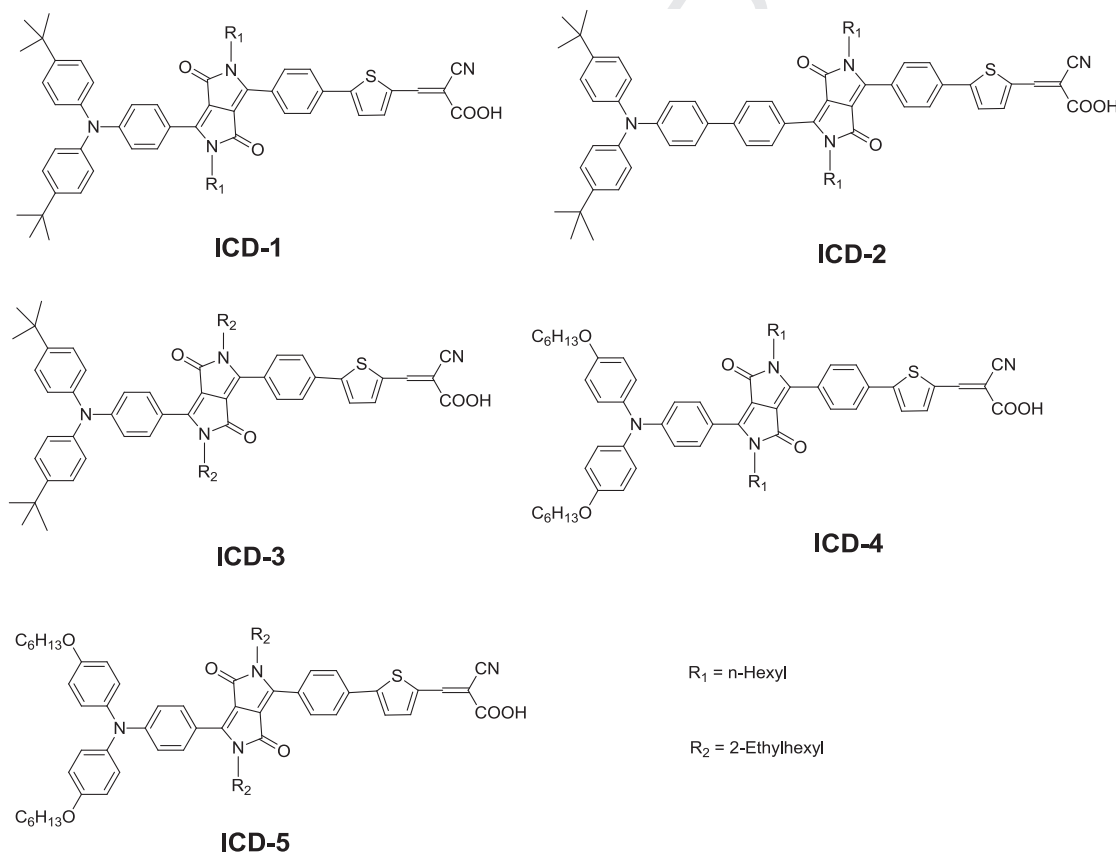
In this article, we further modified the structure of the compact DPP-based dye molecules, and three new DPP dyes, **ICD-3**, **ICD-4**, **ICD-5**, were designed, as shown in Scheme 1. In these dyes, two different substituted triphenylamine donors and different alkyl chains on the periphery of the DPP macrocycle were employed. It was found that **ICD-5** dye with 4-(hexyloxy)-N-(4-(hexyloxy)phenyl)-N-phenylaniline donor and ethyl-hexyl chains showed the

highest power conversion efficiency of 9.10% in DSCs with an I^-/I_3^- based electrolyte under standard AM 1.5 conditions.

2. Experimental section

2.1. Measurement and characterization

NMR spectra were recorded on a BRUKER AVANCE 400 MHz instruments. The residual solvent protons (^1H) or the solvent carbons (^{13}C) were used as internal standards. ^1H NMR data are presented as follows: chemical shift in ppm (δ) downfield from tetramethylsilane (multiplicity, coupling constant (Hz), integration). The following abbreviations are used in reporting NMR data: s, singlet; br. s, broad singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublets; m, multiplet. UV-vis absorption spectra were recorded on a HP 8453 spectrophotometer. Mass spectra were taken on a Bruker Daltonics Inc. APEXII FT-ICR spectrometer. The photocurrent-voltage (I - V) characteristics were recorded at room temperature using a computer-controlled Keithley 2400 source meter under air mass (AM) 1.5 simulated illumination (100 mW cm^{-2} , Oriel, 67,005). The action spectra of monochromatic incident photo-to-current conversion efficiency (IPCE) for solar cells were performed using a commercial setup (PV-25 DYE, JASCO). A 300 W Xenon lamp was employed as light



Scheme 1. Chemical structures of the DPP-based dyes: **ICD-1–ICD-5**.

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