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Effects of the number of chromophores and the bulkiness of a nonconjugated spacer in a dye molecule on the performance of dye-sensitized solar cells

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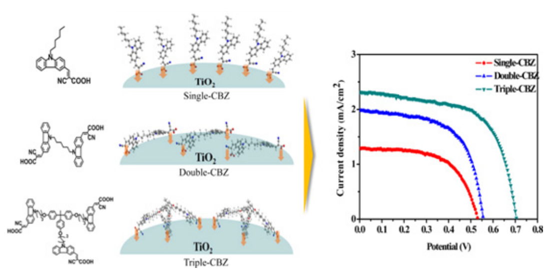
HIGHLIGHTS

- ► Organic dyes with both chromophores and a non-conjugated spacer were synthesized.
- ► The dye with multi-chromophores increased short-circuit current of DSSCs.
- ► The dye with bulkier spacer increased open-circuit voltage of DSSCs.
- ► The bulkier spacer of the dye acted as energy barrier to charge recombination.

GRAPHICAL ABSTRACT



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ABSTRACT

Three organic photosensitizers, Single-, Double- and Triple-CBZ, containing one, two or three carbazole-based chromophores, respectively, and a nonconjugated spacer in each molecule, were designed and successfully synthesized. The electro-optical and photovoltaic properties of the photosensitizers were investigated in terms of molecular microstructure, i.e., the number of the chromophores and the bulkiness of the nonconjugated spacer. A dye-sensitized solar cell (DSSC) based on Triple-CBZ containing three carbazole chromophores and a bulky tris(hexyloxyphenyl)ethane (THPE) spacer showed a considerably improved power conversion efficiency (PCE) of over 55%, mainly due to the enhanced open-circuit voltage (Voc) and short circuit current, when compared with that of the DSSC with Double-CBZ (or Single-CBZ) containing two (or one) carbazole chromophores and a hexyl spacer. More chromophores in the dye molecule increased the molar extinction coefficient, thereby enhancing the energy harvesting efficiency. In addition, a bulkier spacer was favorable for effectively protecting the charge recombination between TiO_2 and electrolytes, thereby improving Voc by the longer electron lifetime.

1. Introduction

Dye-sensitized solar cells (DSSCs) have been widely investigated on account of their special features, such as their low-cost fabrication with fairly high solar energy-to-conversion efficiencies compared to conventional p-n junction solar cells [1,2]. The standard structure of the DSSC comprises an electrochemical cell composed of a dye-adsorbed wide band gap semiconductor electrode, an electrolyte containing I^-/I_3^- redox couples, and a Pt-coated counter electrode [3–5]. The mechanism of the DSSC is based on the injection of electrons from photosensitizers into the conduction band of the electrode on which the photosensitizers are adsorbed. The oxidized photosensitizers are reduced by electron transfer from the electrolyte. With Ru-complex photosensitizers, such as N3 and N719, power conversion efficiencies (PCE) of above 11% have been achieved under AM 1.5 irradiation [6,7], compared to 6 to 9 % for metal-free organic sensitizers [8–13]. Organic dyes are considered as suitable photosensitizers for DSSCs because of their many advantages such as high molar extinction coefficients,

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