DOCTORAL THESIS

Synthesis and characterization of new functional molecules and application studies in dye-sensitized and organic solar cells

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Abstract

This thesis describes the synthesis and characterization of a series of photosensitizers, transition metal-containing polymers and small organic molecules for dye-sensitized solar cells and organic solar cells.

To begin with, a brief overview on the background of dye-sensitized solar cells (DSSCs) and organic solar cells was presented in Chapter 1.

In Chapter 2, a series of novel donor-acceptor-π-acceptor bithiazole-based and fluorenone-based organic dyes for dye-sensitized solar cells were successfully synthesized and fully characterized. We discovered that the performance of the photovoltaic devices depends significantly on the nature and strength of the electron-donating end group along the conjugated main. Some of the materials have been found to show higher power conversion efficiency of 4.71% (V_{oc} = 565 mV, J_{sc} = 11.71 mA cm^{-2}, FF = 0.71) under AM 1.5 irradiation (100 mW cm^{-2}).

In Chapter 3, ten novel donor-donor-π-acceptor organic dyes for dye-sensitized solar cells have been synthesized and applied for the fabrication of DSSCs, including six dibenzothiophene-based photosensitizers and carbazole-based photosensitizers. All the dyes have efficient charge injection from the excited sensitizer molecule to TiO_2 conduction band and can provide ample driving force for efficient dye regeneration

and thus the charge separation. Among all the photosensitizers, DSSCs exhibited the best overall light to electricity conversion efficiency of 5.28% (V_{oc} = 0.70 V, J_{sc} = 11.06 mA cm^{-2}, *FF* = 0.68) under AM 1.5 irradiation, which reached 73% with respect to that of an **N719**-based device fabricated under similar fabrication conditions.

Besides, nine novel di-anchoring organic sensitizers employing two different electron-donating cores, which are the fluorene and carbazole units, and two symmetrical anchoring cyanoacrylic acid (acceptor) termini have been synthesized and studied for their applications in DSSCs in Chapter 4.

In Chapter 5, four new platinum polyyne polymers were prepared *via* the Sonogashira-type dehydrohalogenation reaction between the ethynyl precursor and *trans*-$Pt(PBu_3)_2Cl_2$. All of the polymers are air-stable and well characterized by different spectroscopic methods and photophysical measurements. Their photovoltaic behaviors were fully investigated. Their model compounds were also prepared and studied.

In Chapter 6, a series of new organic small molecules were designed and synthesized comprising head-to-head coupled heylthiophene, dithienosilole and dithienogermole units. They exhibited broad absorption peaks with favorable spectral overlap with the solar spectrum. These seven small molecules have been applied to

the bulk heterojuction solar cells and the corresponding photovoltaic properties were presented. Among these molecules, the highest PCE of 4.93% was achieved with a V_{oc} = 0.79 V, J_{sc} = 1.22 mA cm^{-2} and FF = 0.51 under illumination of an AM 1.5 solar cell simulator.

Finally, Chapters 7 and 8 present the concluding remarks and the experimental details of the work described in Chapters 2−6.

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