DOCTORAL THESIS

Synthesis and characterization of benzodithiophene- and quinoxalinedithienothiophene-based semiconducting materials for organic solar cells

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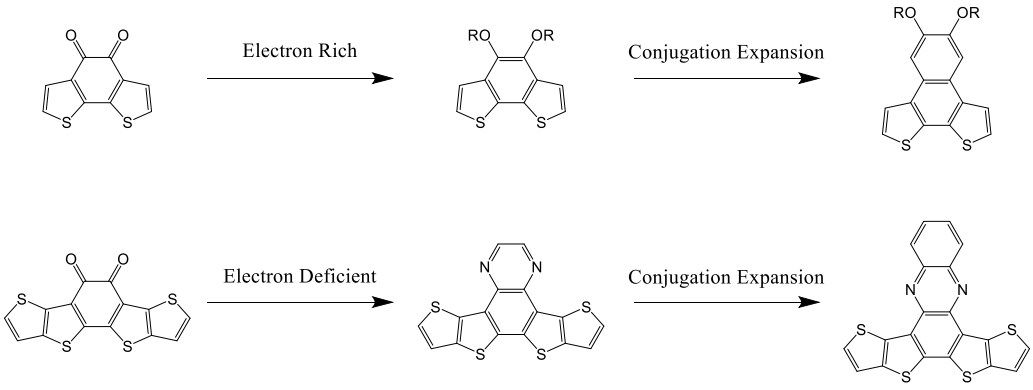
Abstract

Organic semiconducting materials have been attracted considerable attention as a promising technology for the next generation flexible electronic devices, such as solar cells and field-effect transistors because of their advantages of low-cost, structural versatility and flexibility. Many organic semiconducting materials have been developed in recent years.



In this thesis, four π-conjugated building blocks based on benzodithiophene and quinoxalinedithienothiophene were applied to develop novel photovoltaic materials, including donor-acceptor alternating copolymers as a donor material for polymer solar cells, photosensitizers for dye sensitized solar cells, small molecule hole transporting materials for perovskite solar cells and small molecule acceptors for organic solar cells. A comprehensive review of current development of organic photovoltaic materials was presented in Chapter 1.

In Chapter 2, a series of D-A copolymers (**PBB-n**) based on 4,7-di(thiophen-2-yl)benzo[*c*][1,2,5]thiadiazole and 4,5-bis((2-ethylhexyl)oxy)benzo[2,1-*b*:3,4-*b*'] dithiophene attached with different solubilizing side-chains were designed, synthesised and characterized. In general, **PBB-n** polymers showed good absorption in the region of visible light and UV region, indicating such polymers are a promising light harvester.

Also, **PBB-n** exhibited suitable energy levels, suggesting that they could be applied as the donor materials in polymer solar cells. **PBB-n** also exhibited various extent of aggregation behaviour.

Chapter 3 described syntheses and the fluorination effect of two series of fluoro-substituted **PBB-n** copolymers, namely **PfBB-n** and **PffBB-n** on optical, electrochemical, and optoelectronic properties. Among them, **PfBB-n** series was characterized with photovoltaic performance. The champion devices fabricated from **PfBB-12** showed a *PCE* as high as 9.7%, with a V_{oc} of 0.92 V, a J_{sc} of 16.60 mA/cm^{-2} and a *FF* of 63.49%. Cells fabricated from other **PfBB-n** copolymers also exhibited good PV performance with *PCE* ranging from 7.4 – 8.5%. For **PffBB-n** polymers, temperature-dependent aggregation behaviour was exploited by modulating the coating temperature during device fabrication. PSC devices based on **PffBB-n** exhibited good PV performance with *PCE* ranging from 7.4% to 9.9%. Among which, **PffBB-14** provided the most promising PV performance with *PCE* of 9.9%, a V_{oc} of 0.92 V, a J_{sc} of 16.8 mA/cm^{-2} and a *FF* of 64.36%.

Electron deficient conjugated structure was seldom used as the π-bridge in metal-free photosensitizers. In Chapter 4, four novel organic photosensitizers, namely **QC5-m** and **PC5-n** were designed with an electron deficient π-bridge. Typical sandwich-structured DSSCs based on the newly developed photosensitizers exhibited promising photovoltaic performance with *PCE* ranging from 5.23 – 7.77 %, with a maximum J_{sc} as high as 15.63 mA cm^{-2}. These results suggest that the use of electron deficient π-bridge provides alternative approach to construct efficient organic photosensitizers.

Chapter 5 and Chapter 6 described the design, synthesis and investigation of novel hole-transporting materials and electron acceptor materials based on benzo[2,1-*b*:3,4-

b']dithiophene-4,5-dione derived building blocks as potential organic photovoltaic materials for solar cell applications.

Keywords: organic photovoltaic materials, photosensitizers, polymer solar cell, electron acceptor, hole-transporting materials.

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