

DOCTORAL THESIS

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

Huang, Lanqi

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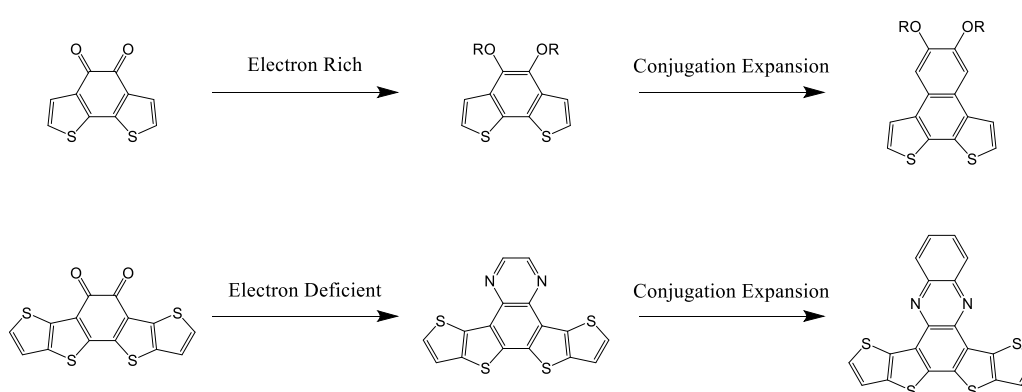
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Abstract

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.

TABLE OF CONTENTS

DECLARATION	i
ABSTRACT	ii
FORMULA INDEX	vi
DECLARATION	i
ABSTRACT	ii
FORMULA INDEX	v
ACKNOWLEDGEMENTS	viii
LIST OF SCHEMES	xv
LIST OF TABLES	xvi
LIST OF FIGURES	xix
LIST OF ABBREVIATIONS AND SYMBOLS	xxv
CHAPTER ONE	1
ORGANIC PHOTOVOLTAIC CELLS: INTRODUCTION AND RECENT DEVELOPMENTS	1
1.1 INTRODUCTION TO ORGANIC SOLAR CELLS.....	1
1.1.1 General Background	1
1.1.2 Working Principle of Organic Solar Cells.....	2
1.1.3 Basic Photovoltaic Concepts	3
1.2 INTRODUCTION TO BULK HETEROJUNCTION SOLAR CELLS	6
1.2.1 Introduction	6
1.2.2 Operational Mechanism of Bulk Heterojunction Solar Cells.....	7

1.2.3 Recent Development of Donor Polymer Materials	9
Effect of side chain on device performance	10
Effect of polymer backbone structures	13
Aggregation and crystallization ability.....	15
1.2.4 Recent Developments in SMAs.....	17
1.2.5 Summary and Motivation	21
1.3 INTRODUCTION TO DYE-SENSITIZED SOLAR CELLS	22
1.3.1 Introduction	22
1.3.2 Operational Mechanism of DSSCs.....	22
1.3.3 Recent Developments in DSSCs	23
General design strategy of dyes.....	25
Donor units	25
The π -bridges.....	27
Acceptor/anchor group	29
1.3.4 Summary and Motivation	30
1.4 INTRODUCTION TO PEROVSKITE SOLAR CELLS	31
1.4.1 Introduction	31
1.4.2 Operational Mechanism of Perovskite Solar Cells.....	31
1.4.3 Recent Development of Organic HTMs.....	33
Alternating donor–acceptor structure in HTMs.....	33
Linear/discotic/star-shaped HTMs	35
3D/spiro-configured HTMs	39
1.4.4 Summary and Motivation	42
CHAPTER TWO.....	43

IMPACT OF ALKYL CHAIN LENGTH OF BENZODITHIOPHENE- BENZOTHIADIAZOLE BASED COPOLYMERS	43
2.1 INTRODUCTION	43
2.2 RESULTS AND DISCUSSION	44
2.2.1 Synthesis.....	44
Synthesis of Donor Unit	44
Synthesis of Acceptor Units	45
Synthesis of Polymers	46
2.2.2 Optical and Electrochemical Properties of PBB-n Polymers	48
2.3 CONCLUSIONS.....	52
2.4 EXPERIMENTAL SECTION	53
2.4.1 General Characterization of Materials.....	53
2.4.2 Synthetic Procedure.....	54
CHAPTER THREE.....	64
FLUORINATION EFFECT OF BENZODITHIOPHENE- BENZOTHIADIAZOLE BASED LOW-BAND GAP COPOLYMERS.....	64
3.1 INTRODUCTION	64
3.2 RESULTS AND DISCUSSION	66
3.2.1 Synthesis.....	66
Synthesis of Donor Unit	66
Synthesis of Acceptor Units	66
Synthesis of Polymers	68
3.2.2 Optical and Electrochemical Properties of PfBB-n Polymers.....	70
3.2.3 Device Performance of PfBB-n Polymers.....	74

Photovoltaic Performance.....	74
Electron Transfer and Recombination.....	77
Morphological Study	80
3.2.4 Optical and Electrochemical Properties of PffBB-n Polymers	81
3.2.5 Device Performance of PffBB-n Polymers	84
Photovoltaic Performance.....	84
Electron Transfer and Recombination.....	87
Morphological Study	90
3.3 CONCLUSIONS.....	91
3.4 EXPERIMENTAL SECTION	93
3.4.1 General Characterization of Materials.....	93
3.4.2 Cell Fabrication	94
3.4.3 Device Characterization	94
3.4.4 Synthetic Procedure.....	96
CHAPTER FOUR	106
SYNTHESIS AND CHARACTERIZATION OF NOVEL QUINOXALINE AND	
PHENAZINE BASED ORGANIC DYES FOR DYE SENSITIZED SOLAR CELL	
APPLICATION	106
4.1 INTRODUCTION	106
4.2 RESULTS AND DISCUSSION	108
4.2.1 Synthesis.....	108
Synthesis of Donor Unit	108
Synthesis of Acceptor Units	109
Synthesis of Photosensitizers	111
4.2.2 Thermal Properties	113

4.2.3 Optical and Electrochemical Properties	113
4.2.4 Device Optimization and Performance.....	120
Device Optimization.....	120
Photovoltaic Performance.....	126
Charge Transfer and Recombination.....	128
4.3 CONCLUSION	132
4.4 EXPERIMENTAL SECTION	133
4.4.1 General Characterization of Materials.....	133
4.4.2 Cell Fabrication	134
4.4.3 Device Characterization	134
4.4.4 Synthetic Procedure.....	135
CHAPTER FIVE	155
BENZODITHIOPHENE- AND NAPHTHODITHIOPHENE-BASED HOLE-	
TRANSPORTING MATERIALS FOR PEROVSKITE SOLAR CELLS	155
5.1 INTRODUCTION	155
5.2 RESULTS AND DISCUSSION	156
5.2.1 Synthesis.....	156
5.2.2 Thermal Properties of HTMs.....	158
5.2.3 Optical and Electrochemical Properties	159
5.2.4 Device Performance of HTMs.....	163
5.3 CONCLUSIONS.....	164
5.4 EXPERIMENTAL SECTION	165
5.4.1 General Characterization of Materials.....	165
5.4.2 Synthetic Procedure.....	166

CHAPTER SIX.....	173
BENZODITHIOPHENE AND QUINOXALINEDITHIENOTHIOPHENE DERIVATIVES FOR CONSTRUCTION OF SMALL MOLECULE ACCEPTORS	173
6.1 INTRODUCTION	173
6.2 RESULTS AND DISCUSSION	174
6.2.1 Synthesis.....	174
Synthesis of Naphthodithiophene-Based Acceptors	174
Synthesis of Quinoxaline and Phenazine Cored Acceptors.....	176
6.2.2 Thermal Properties of SMAs.....	177
6.2.3 Optical and Electrochemical Properties	177
6.3 CONCLUSIONS.....	181
6.4 EXPERIMENTAL SECTION	182
6.4.1 General Characterization of Materials.....	182
6.4.2 Synthetic Procedure.....	183
CHAPTER SEVEN	192
CONCLUDING REMARKS.....	192
APPENDIX I ¹H NMR SPECTRA OF SELECTED COMPOUNDS	195
APPENDIX II ¹³C NMR SPECTRA OF SELECTED COMPOUNDS	202
APPENDIX III MASS SPECTRA OF SELECTED COMPOUNDS.....	207
LIST OF PUBLICATION	217
REFERENCE	218
CURRICULUM VITAE	227