

DOCTORAL THESIS

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

Lai, Lai Fan

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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 TiO₂ 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 polyene polymers were prepared *via* the Sonogashira-type dehydrohalogenation reaction between the ethynyl precursor and *trans*-Pt(PBu₃)₂Cl₂. 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 heterojunction 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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Table of contents

Declaration	i
Abstract	ii
Acknowledgements	v
Table of Contents	viii
List of Tables	xvii
List of Figures	xx
List of Schemes	xxxii
List of Charts	xxxvi
List of Abbreviations and Symbols	xli
Formula Index	xlii
Chapter 1 Introduction	1
1.1 Dye-sensitized Solar Cells (DSSCs)	1
1.1.1 Background	1
1.1.2 Operation Principle of Organic Solar Cells	2
1.1.2.1 Overview of the Different Electron-Transfer Processes	5
1.1.2.2 Reactions 1 and 2: Electron Injection and Excited State Decay	6

1.1.2.3	Reaction 3: Regeneration of the Oxidized Dyes	7
1.1.2.4	Reaction 4: Electron Transport through the Mesoporous Oxide Film	8
1.1.2.5	Reactions 5 and 6: Recombination of Electrons in the Semiconductor with Oxidized Dyes or Electrolyte Species	8
1.1.2.6	Reaction 7: Reduction of Electron Acceptors in the Electrolyte at the Counter Electrode	9
1.1.3	Efficiency Measurements	9
1.1.3.1	Measurement of $I-V$	9
1.1.3.2	Measurement of IPCE	11
1.2	Organic Solar Cells	12
1.2.1	Background	12
1.2.2	Structure and Operation Principle of Organic Solar Cells	14
1.2.3	Conjugated Polymer Cells	18
1.2.4	Small Molecules	21
1.3	Scope of the Thesis	24
	References	25

Chapter 2 Novel Donor-Acceptor- π -Acceptor Organic

	Dyes for Dye-sensitized Solar Cells	30
2.1	Synthesis and Characterization of Functionalized Bithiazole-based Dye-sensitized Solar Cells	30
2.1.1	Introduction	30
2.1.2	Synthesis	33
2.1.3	Results and Discussion	37
	2.1.3.1 Spectroscopic Characterization	37
	2.1.3.2 Photophysical Properties	39
	2.1.3.3 Electrochemical Properties	43
	2.1.3.4 Computational Studies	45
2.1.4	Applications in DSSCs	52
	2.1.4.1 Preparation of DSSC Devices	52
	2.1.4.2 Photovoltaic Performance of DSSCs	53
2.1.5	Cytotoxicity Test of Dye-sensitizers on Human Cells	60
2.2	Synthesis and Characterization of Fluorenone-containing Organic Photosensitizers for Dye-sensitized Solar Cells	63
2.2.1	Introduction	63
2.2.2	Synthesis	66
2.2.3	Results and Discussion	69

2.2.3.1	Photophysical Properties	69
2.2.3.2	Electrochemical Properties	73
2.2.3.3	Computational Studies	75
2.2.4	Applications in DSSCs	77
2.2.4.1	Preparation of DSSC Devices	77
2.2.4.2	Photovoltaic Performance of DSSCs	79
2.3	Concluding Remarks	85
	References	87
Chapter 3	New Donor-Donor-π-Acceptor Organic Dyes for Dye-sensitized Solar Cells	97
3.1	Synthesis and Characterization of Functionalized Dibenzothiophene-based Dye-sensitized Solar Cells	97
3.1.1	Introduction	97
3.1.2	Synthesis	99
3.1.3	Results and Discussion	103
3.1.3.1	Spectroscopic Characterization	103
3.1.3.2	Photophysical Properties	105
3.1.3.3	Electrochemical Properties	109
3.1.3.4	Computational Studies	112

3.1.4	Applications in DSSCs	118
	3.1.4.1 Preparation of DSSC Devices	118
	3.1.4.2 Photovoltaic Performance of DSSCs	119
3.2	Synthesis and Characterization of Functionalized Carbazole-based Dye-densitized Solar Cells	125
3.2.1	Introduction	125
3.2.2	Synthesis	127
3.2.3	Results and Discussion	131
	3.2.3.1 Spectroscopic Characterization	131
	3.2.3.2 Photophysical Properties	132
	3.2.3.3 Electrochemical Properties	135
	3.2.3.4 Computational Studies	138
3.2.4	Applications in DSSCs	141
	3.2.4.1 Preparation of DSSC Devices	141
	3.2.4.2 Photovoltaic Performance of DSSCs	143
3.3	Concluding Remarks	149
	References	151

Chapter 4 Novel Symmetrical Di-anchoring Organic Photosensitizers for Dye-sensitized Solar

	Cells	160
4.1	Introduction	160
4.2	Synthesis	162
4.3	Results and Discussion	166
4.3.1	Spectroscopic Characterization	166
4.3.2	Photophysical Properties	168
4.3.3	Electrochemical Properties	172
4.4	Applications in DSSCs	175
4.4.1	Preparation of DSSC Devices	175
4.4.2	Photovoltaic Performance of DSSCs	177
4.5	Concluding Remarks	182
	References	184
Chapter 5	Synthesis and Characterization of Novel Metallopolyyne Polymers as New Functional Materials for Application in Solar Cells	187
5.1	Introduction	187
5.2	Synthesis	190
5.3	Results and Discussion	194
5.3.1	Spectroscopic Characterization	194

5.3.2	Photophysical Properties	199
5.3.3	Electrochemical Properties	204
5.3.4	Molecular Weight Determination of Metallopolyyne Polymers	206
5.5	Applications in Polymer Solar Cells (PSCs)	207
5.6	Concluding Remarks	216
	References	217
Chapter 6	Novel Small Molecules for Bulk Heterojunction Solar Cells	221
6.1	Introduction	221
6.2	Synthesis	223
6.3	Results and Discussion	229
6.3.1	Computational Studies	229
6.3.2	Spectroscopic Characterization	233
6.3.3	Thermal Properties	240
6.3.4	Photophysical Properties	243
6.3.5	Electrochemical Properties	245
6.3.6	XRD Studies	250
6.4	Application in BHJ Solar Cells	253

6.5	Concluding Remarks	258
	References	260
Chapter 7	Concluding Remarks and Future Work	263
Chapter 8	Experimental Details	270
8.1	General	270
8.2	Materials	274
8.3	Experimental Details for Chapter 2	275
8.3.1	Experimental Details for Various Boronic Acid Derivatives	275
8.3.2	Experimental Details for Halide Precursors	279
8.3.3	Experimental Details for Aldehyde Precursors	289
8.3.4	Experimental Details for Dyes	296
8.4	Experimental Details for Chapter 3	300
8.4.1	Experimental Details for Various Boronic Acid Derivatives	300
8.4.2	Experimental Details for Halide Precursors	301
8.4.3	Experimental Details for Aldehyde Precursors	316
8.4.4	Experimental Details for Dyes	322

8.5	Experimental Details for Chapter 4	326
8.5.1	Experimental Details for Various Boronic Acid Derivatives	326
8.4.2	Experimental Details for Halide Precursors	330
8.4.3	Experimental Details for Aldehyde Precursors	334
8.4.4	Experimental Details for Dyes	340
8.6	Experimental Details for Chapter 5	344
8.6.1	Experimental Details for Halide Precursors	344
8.6.2	Experimental Details of Sonogashira Coupling (Synthesis of L1-TMS to L4-TMS)	352
8.6.3	Experimental Details of the Deprotection of Trimethylsilyl Group (Synthesis of L1-L4)	355
8.6.4	Experimental Details of Polymers	357
8.6.5	Experimental Details for Model Compounds	358
8.7	Experimental Details for Chapter 6	362
8.7.1	Experimental Details for Core Materials	362
8.7.2	Experimental Details for Halide Precursors	364
8.7.3	Experimental Details for Stannylated Precursors	367
8.7.4	Experimental Details for Small Molecules	381
	References	387

