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Molecular Design of New Small Molecules and Polymers: Synthesis, Characterization and Application in Organic Solar Cells

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A thesis submitted in partial fulfillment of the requirements

for the degree of

Doctor of Philosophy

Principal Supervisor: Professor WONG Wai Yeung, Raymond

Hong Kong Baptist University

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Abstract

The molecular design, synthesis, spectroscopic and photophysical characterization of a new series of organic small molecules and transition metal-containing polymers incorporating different π-conjugated chromophores are discussed. The applications of some of these compounds in bulk heterojunction (BHJ) organic solar cells are also outlined.

Chapter 1 contains a brief overview on the background of organic solar cells, their structures and performance in solution-processed organic BHJ devices.

Chapter 2 presents the synthetic methodology and characterization of a series of new dipyrrin-based materials and their application in organic solar cells. In this section, four metal-based metallopolymers for organic solar cells have been designed, synthesized and two of them have been fabricated for BHJ organic solar cells. Through the alternation of different metal ions and boron element in the same dipyrrin framework, a series of dipyrrin-based metal complexes and BODIPY-containing compounds have been synthesized. Electrochemical analysis and DFT calculations proved that **M4** with BODIPY-based structure is more efficient in optimizing the HOMO-LUMO energy level which further increases the V_{oc} value.

A full account of the preparation, characterization, photophysical and thermal

properties of a new series of benzo[1,2-*b*:4,5-*b′*]dithiophene (BDT), cyclopenta[2,1-*b*:3,4-*b′*]dithiophene (CPT) and triphenylamine (TPA) centered small molecules are presented in chapters 3, 4 and 5, respectively. Different acceptor-donor-acceptor (A-D-A) based materials were prepared and employed in organic solar cells in order enhance the power conversion efficiency (PCE) of the devices. Some of the materials have been found to show higher PCEs of up to 3.91%. Given the excellent solution-processability as well as performance advantage, this work provides us a feasible strategy to develop low-cost and high PCE materials in solar cell applications, which would help small molecular organic solar cells to reach a level of practical applications.

In chapter 6, four low-bandgap Pt-containing polymers were synthesized and characterized by a variety of techniques. Among them, the largest λ_{onset} of 699 nm in solution and λ_{onset} of 736 nm in the thin film of **P6** were observed and the corresponding energy gap E_g was estimated to be 1.77 eV and 1.68 eV, respectively. After evaluating these oxidation and reduction potentials, **P6** also showed the smallest band gap of 1.65 eV with the corresponding HOMO and LUMO energy levels of -5.17 eV and -3.52 eV, respectively. Also, the molecular weights of these polymers were examined by the GPC method. The highest M_n of 24.0 kDa and M_w of 50.4 kDa with the PDI of 2.10 were observed in **P8**.

Chapter 7 and 8 present the concluding remarks and the experimental details of the work described in Chapters 2-6.

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