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

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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 \( \lambda_{\text{onset}} \) of 699 nm in
solution and \( \lambda_{\text{onset}} \) 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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