DOCTORAL THESIS

# Synthesis, characterization and optoelectronic applications of new conjugated organic and organometallic polymers

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*Date of Award:*
2011

# Synthesis, Characterization and Optoelectronic Applications of New Conjugated Organic and Organometallic Polymers

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**A thesis submitted in partial fulfillment of the requirements**

**for the degree of**

**Doctor of Philosophy**

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**May 2011**

# Abstract

Polymer solar cells have attracted considerable attention for the potential application as renewable energy sources due to their unique advantages of the ease of solution-processing, low cost, light weight and flexible large-area devices, and encouraging progress has been made in the past decade. Metal-containing conjugated polymers represent an intriguing and promising class of materials, and platinum polyyne polymers have been shown to be good candidates for organic solar cells. Organic conjugated polymers as the other important type of materials have also been extensively studied in the field of solar cells, and show outstanding performance.

New series of metal-containing polymers based on different π-conjugated chromophores and a new type of organic conjugated polymers with lower band gaps were synthesized and fully characterized. The applications of some of these polymers in solar cells or field-effect transistors are also outlined.

Chapter 1 contains a brief overview on the background, basic theory and development of bulk-heterojuction (BHJ) solar cells.

Chapter 2 presents the synthesis and characterization of a new series of platinum(II)-containing conjugated polymers based on pyran, diketopyrrolopyrrole, benzothiadiazole or thiadiazolo[3,4-*c*]pyridine, fluorene and phenanthrenyl-imidazole chromophores, typically designed via a donor-acceptor (D-A) approach. These polymers were synthesized by Sonogashira-type dehydrochloride reaction between the diethynyl ligands and *trans*-$Pt(PBu_3)_2Cl_2$. Their photophysical properties were

fully investigated by the UV-vis and PL spectroscopies. In addition, the HOMO and LUMO energy levels of all the polymers were tested by cyclic voltammetry. The band gap of polymers can be tuned by changing the electron-donating ability of donor unit or the electron-withdrawing ability of acceptor unit in a D-A system. Some of the platinum polyyne polymers have been fabricated into photovoltaic devices and showed the power conversion efficiency (PCE) up to 1.4%.

A full account of the preparation, characterization, photophysical and thermal properties of a new series of organometallic polymers based on zinc(II)-porphyrin and platinum(II) alkynyls are presented in Chapter 3. These polymers exhibit a strong Soret band at ca. 430 nm and two weak Q-bands between 540 nm and 635 nm, which is a typical absorption profile for porphyrin compounds. The frontier molecular orbitals for their corresponding oligomeric model compounds were fully investigated by DFT and TDDFT. Photovoltaic devices based on theses polymers were fabricated and showed good photovoltaic performance.

In Chapter 4, a new series of organic conjugated polymers based on cyclopentadithiophene and thiadiazolo-[3,4-*c*]pyridine or pyridine were designed and synthesized by the novel microwave-assisted Stille-coupling reaction. Most of these polymers show better absorption properties in the visible and near-infrared region. The charge carrier mobilities of some of them were investigated by organic field-effect transistors. This series of polymers showed higher charge carrier mobilities, the highest value reaching up to 0.022 $cm^2\ V^{-1}\ s^{-1}$ for hole mobility and 0.12 $cm^2\ V^{-1}\ s^{-1}$ for electron mobility, presented by the regioregular polymer **P21**.

Chapters 5 and 6 present the concluding remarks and the experimental details of the work described in Chapters 2–4.

## Table of Contents