

## DOCTORAL THESIS

# Structural engineering of porphyrin small molecules for bulk heterojunction organic solar cell applications

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## Abstract

Organic donor and acceptor have promised the better future energy technologies to alleviate global energy demand and environmental issues. And nowadays they begin to come true in bulk heterojunction organic solar cells (BHJ OSCs) with advantages of low-cost, light-weight, large-area, flexibility, and with high efficiencies (PCEs) of over 14% for converting solar energy to electricity. Porphyrins are unique potential for artificial photocatalysis but their application in BHJ OSCs are still limited by the PCEs less than 10%. This complicacy comes from their inadequate spectral absorptions and the imperfect morphologies. In this thesis, we devote to chemical modification of acceptor- $\pi$ -porphyrin- $\pi$ -acceptor (A- $\pi$ -Por- $\pi$ -A) structural molecules to enhance their spectral absorptions and phase-separation functions with fullerene acceptor. Firstly, chemically driving *J*-aggregates have been studied on the new A- $\pi$ -Por- $\pi$ -A porphyrin molecule, which could improve the phase-separation of its blend film with PC<sub>71</sub>BM and enhance its performance in BHJ OSCs with PCE up to 8.04%. Secondly, two new benzodithiophene (BDT)  $\pi$ -bridged A- $\pi$ -Por- $\pi$ -A molecules have been prepared with complementary absorption between the Soret and Q bands. The devices based on the blend films of the porphyrin donor and PC<sub>71</sub>BM acceptor exhibit full spectral photocurrent generation and impressive PCEs up to 7.92%. Thirdly, we further extended the  $\pi$ -conjugation of the above BDT  $\pi$ -bridged A- $\pi$ -Por- $\pi$ -A molecules by inserting alkyl chain substituted thiophene derivatives into their backbones, resulting in new porphyrin molecules with UV-visible-near-infrared

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absorption spectra. Using those porphyrin molecules as donor and PCBM as acceptor, the devices show full spectra photocurrent generation and appropriate film morphology, resulting in high PCE up to 8.59%.

Besides, photocatalysis is also a new promising technology to generate renewable energy. We herein develop new low-cost and noble-metal-free photocatalysts based on Co(OH)<sub>2</sub> modified CdS nanowires and applied them for visible light driven hydrogen production from water-splitting. The optimum H<sub>2</sub> production rate reaches 14.43 mmol·h<sup>-1</sup>·g<sup>-1</sup> under ( $\lambda \geq 420$  nm) upon visible light irradiation, which is 206 and 3 times larger than that of the pristine CdS NWs and 1 wt% Pt-CdS NWs, respectively. The results indicate the promising application of earth-abundant Co(OH)<sub>2</sub> as alternative cocatalysts of noble metals.

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