DOCTORAL THESIS

New molecular materials for organic and dye-sensitized solar cells and photocatalytic hydrogen generation

Ho, Po Yu

Date of Award:
2016

Abstract

Emerging solar energy technology, including photovoltaics, solar fuels generation and solar thermal systems, is considered as one of the most potential renewable energy resources because of the tremendous and free radiant energy supply by our sun. Unlike burning of fossil fuels, carbon dioxide emission-free energy conversion process is definitely another key feature and attracting scientists to explore these research areas. Besides, this implies a giant business market to compete with traditional fossil fuel companies. Nevertheless, it is too early to realize commercial application since the technologies are in the early development stage and there is still much room to explore and improve. Simply speaking, energy conversion efficiency, robustness, environmental impacts and cost are the major factors the community should deeply concentrate on at this moment. This provides many research opportunities on the creation of novel molecular functional materials and investigates the relationship between the molecular design and functional properties, and they obviously take up significant roles in the technology evolution.

The basic concepts and conspectuses regarding organic photovoltaics and light-driven hydrogen generation are collected in Chapter 1.

In Chapter 2, a series of new thiophene-based small molecules is presented and the discussion is focused on its application in the bulk-heterojunction organic solar cells. Importantly, the structure-property relationship is elucidated by varying the terminal electron withdrawing group and elongating the central electron donating unit. The highest power conversion efficiency (η) of 2.6% is attained by the device with compound **M3** as the active material with traditional device configuration (without any annealing process and additives addition) under AM 1.5G irradiation.

In Chapter 3, a series of D−π−A organic dyes is introduced and the discussion concentrates on its application in the dye-sensitized solar cells. Briefly, a case study on alkyl chain effects is investigated while a new starburst triarylamine donor and uncommon selenophene-containing π-linker are studied separately. The highest power conversion efficiency (η) of 6.7% is achieved by **D11** under AM 1.5G irradiation with a high open-circuit voltage of 0.825 V.

In Chapter 4, three new platinum(II) diimine complexes are synthesized and they are utilized as photosensitizers with platinized titanium dioxide as catalyst site in the context of light-driven hydrogen generation. Comparison between platinum(II) diimine dithiolate complex and platinum(II) diimine bis(acetylide) complex is accomplished, and the importance of photosensitization using an organic chromophore with a desirable energy transfer consideration is accounted.

Finally, Chapter 5 puts forward the concluding remarks and possible future works while Chapter 6 includes all the experimental details of the studied compounds presented in Chapter 2−4.

Table of Contents