DOCTORAL THESIS

Metallated and metal-free molecular dyes for dye-sensitized solar cells

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Abstract

The molecular design, synthesis and spectroscopic characterization of a series of ruthenium(II), metal-free and platinum(II) photosensitizers were discussed. The applications of some of these compounds in dye-sensitized solar were also outlined.

To start with, a brief overview on the background of dye-sensitized solar cells (DSSCs) was presented in Chapter 1.

In Chapter 2, a series of new thiocyanate-free ruthenium(II) cyclometalated complexes with different ligands were successfully synthesized and some of them were fully characterized by spectroscopic and computational methods. The nature of cyclometalating ligands effectively tunes the properties of the metal complexes and the resulting DSSC performance.

In Chapter 3, new di-anchoring organic dyes have been synthesized and characterized. This molecular design strategy can significantly enhance the η value because this successfully inhibits the undesirable charge combination and prolongs the electron lifetime. The discoveries open up a new avenue to the evolution of organic sensitizers and the optimization of bridged di-anchoring dyes for highly efficient co-adsorbent-free DSSCs.

In Chapter 4, a series of new thiophene-free platinum sensitizers for the application

of DSSCs was developed. Four unsymmetrical platinum(II) di-acetylide complexes containing phenothiazine moiety with different donor units were designed and synthesized. These photosensitizers were fully characterized by spectroscopic as well as computational studies and also successfully employed in DSSC fabrication. These findings provided positive evidence that platinum-acetylide complexes have a great potential and prospect for the use as promising metal-based photosensitizers in DSSC applications.

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

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