Abstract

Dye-sensitized solar cells (DSSC) have attained considerable attention during the last decade because of the potential of becoming a low cost alternative to silicon based solar cells. Although efficiencies exceeding 10% in full sunlight have been presented, major improvements of the system are however limited. Phthalocyanines are an important class of high performance compound, which are easily processable, and display good mechanical properties, outstanding thermal and thermal-oxidative stability. This thesis present theoretical study of some metal substituted Phthalocyanine dye sensitizer for solar energy conversion applications using quantum calculation methods.

The first chapter was a general introduction to the photovoltaics and dye-sensitized solar cells, such as the operating principles and the characteristics of the dye cell.

In Chapter 2, we specified the theoretical backgrounds and importance of the Phthalocyanine dyes for solar cell applications.

From Chapter 3 to Chapter 7, we studied the performance of six metal substituted Phthalocyanine (MPc) organic sensitizer in DSSC. The geometries, HOMO, LUMO and HOMO-LUMO energy gap of MPc dye sensitizers were studied based on DFT and HF method using the hybrid

functional B3LYP. UV-Vis spectra were investigated by DFT and HF method methods and also the results are analyzed.

We drew some final concluding remarks in Chapter 8 with brief short discussion and also plan of future research works for dye-sensitized solar cell applications.

Key words: Metal substituted Phthalocyanine (MPc), DFT and HF method, HOMO-LUMO energy gap, UV-Vis spectra.