Abstract

In this thesis, merocyanine (MC) dyes are applied in combination with fullerene based acceptors in organic solar cells (OSC). Due to their intense and tunable absorption as well as their electronic structure, MCs are promising candidates as donor materials for highly efficient photovoltaic devices. Previous studies revealed rather large currents and voltages for MC based bulk heterojunction (BHJ) device architectures. However, the solar cell efficiencies are limited by poor fill factors. The thesis at hand addresses mercocyanine based solar cells at different length scales, i.e. the molecular level, supramolecular level, bulk heterojunction level and device level. The results allow to identify the key elements needed to improve the performance of MC based solar cells.

The influence of the heteroatom in the donor subunit of merocyanines is explored by photoelectron spectroscopy and is correlated to the bond length alternation in the single-crystal as well as to the absorption in the thin film. The results show that the appearance of MCs in thin films is dominated by their zwitterionic resonance structure but close to the cyanine limit.

The implementation of a newly designed bis(merocyanine) as donor in BHJ devices leads to exceptional photocurrent generation in highly aggregated π-stacks. Efficiencies exceeding that of the solar cell with the corresponding MC are obtained due to enhanced absorption and charge carrier mobility in the aggregated domains. The concomitant reduction of open-circuit voltage when aggregated domains of MCs are present is subsequently investigated in more detail.

The inferior performance of contaminated MC batches is traced back to impurities, which act as traps for charge carriers and quench excitons. Intensity dependent measurements indicate that BHJ solar cells with merocyanines suffer from severe geminate as well as bimolecular recombination.

An applied new method to tune the work function of the hole collecting contact reveals a dependency of the open-circuit voltage on the height of injection barrier. Finally, a new simple technique to determine the optical constants of bulk heterojunction active layer materials from standard solar cell measurements is developed.