Abstract

In recent years, organic solar cells have attracted great attention as a technology that can convert sunlight into electricity. Since production and material costs are very low, they represent a promising alternative to common solar cells. However, organic solar cells suffer from moderate power conversion efficiencies. Predictable correlations between the molecular structure or properties and the device performance are mandatory to further drive the progress in this area. To obtain structure-property correlations, 21 structurally related merocyanine dyes were studied as donor component with the acceptor C_{60} in organic solar cells. The devices were fabricated by physical vapour phase deposition under high-vacuum conditions.

In the first part of this thesis the influence of the molecular structure of merocyanine dyes on the optical and electrical properties of the solar cells was studied. It was shown that the open-circuit voltage scales linearly with the highest occupied molecular orbital of the donor whereas the short-circuit current is determined by the difference between the lowest molecular orbitals of the donor and acceptor. Moreover, the characteristic packing motifs of merocyanine dyes in single crystals were analysed and found to correlate with the fill factor of the solar cells.

In the second part of this thesis the origin of the open-circuit voltage of planar and bulk heterojunction solar cells was analysed. It was shown that the effective photovoltaic energy gap is the upper limit for the open-circuit voltage and can be determined from temperature and light intensity depended current-voltage curves of a solar cell. However, only the analysis of the current-voltage curves measured under illumination has led to reliable results since the dark current was found to be highly affected by trapping of charge carriers in deep trap states. In addition, the effective photovoltaic energy gap was found to depend on the device architecture.

In the last two parts of this thesis the morphology of pure merocyanine layers and various donor-acceptor blends was studied. It was shown that the power conversion efficiency of merocyanine-fullerene bulk heterojunction solar cells can be significantly increased by integrating a thin crystalline contact layer. Furthermore, small-angle neutron scattering is introduced to probe the morphology of pure and blend thin films of small molecules.