Carbon Nanotube Based Efficiency Enhancement and Numerical Modelling of Organic Bulk Heterojunction Solar Cells

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Abstract

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This thesis covers both experimental and modelling work regarding the organic solar cells. The performance of organic solar cells is often hampered by the poor charge extraction from the device active layer. The experimental section of the this research work deals with enhancing the extraction of the photo-generated charge carriers from the active layer which would lead towards better device efficiency values. Single walled carbon nanotubes are the charge extractors of choice in this work, and two distinct approaches are employed for incorporating the carbon nanotubes to the devices. The first approach is based on the previous work of similar manner and is investigated using devices based on well a characterized active layer polymer blend Poly(3-hexylthiophene-2,5-diyl)(P3HT) and [6,6]-Phenyl-C61-butyric acid methyl ester ($PC_{60}BM$). The second approach presented is novel and derived to overcome the shortcomings of the first approach. This approach is investigated using devices based on a newer and much better performing polymer blend Poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl]] (PTB7) and [6,6]-Phenyl-C71-butyric acid methyl ester ($PC_{70}BM$).

The second part of this thesis deals with modelling of organic solar cells. A fundamental physics based numerical model is derived for donor acceptor polymer based bulk heterojunction organic solar cells. The derived model focuses on the optical absorption and charge extraction of the modelled device. The model is capable of predicting the device performance for different device architectures, different active layer polymer blends and different charge extraction layers and end contacts as well. Using the de-

in detail for both optical and electrical performance, and the active layer thickness optimization is carried out. The model is used to investigate the effect of absorption profile shape, charge carrier mobility of each type of charge carrier and device architecture on the device performance and the suitable device architectures for each polymer blend mentioned above have been identified for the best device performance. In addition the model is used to investigate the impact of performance enhancement techniques such as optical spacers and charge extraction layers and their effect on both device optical performance and overall device performance have been quantified.