Charge transfer process in active layer of organic solar cells

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The aim of this thesis are comprehensive studies of exciton formation and separation to free electrons and holes through charge transfer (CT) occurring in active layer of organic solar cells, together with understanding of physical mechanisms essential for these processes. An importance of such studies can be justified by constantly growing interest in renewable energy sources, particularly - photovoltaics.

Chapter 1 presents properties of materials used in organic solar cells, individually for polymer and perovskite devices. Working principles of such photocells are also described. In the case of polymer solar cells, special attention is given to the processes of exciton creation and separation through CT.

Next Chapter consists of brief overview of materials for polymer and perovskite photovoltaics, together with more extended description of materials studied in this thesis. Polymers belonging to poliazomthine group were used as donor material. It is noteworthy, that synthesis of such compounds is simple and cheap. As reference donor materials commercially available polymers shortly named P3HT and PCDTBT were chosen. The fullerene derivative was used as acceptor.

Applied experimental methods are presented in Chapter 3. Among others, absorption spectroscopy providing information for photon energy range necessary for exciton creation is described, together with two spectroscopic techniques, namely, time-resolved photoluminescence (TRPL) and light-induced electron spin resonance (LESR), which we found especially useful for direct detection of CT phenomenon. Experimental results were supported by theoretical calculations of HOMO (the highest occupied molecular orbital) and LUMO (the lowest occupied molecular orbital) levels of polymers and fullerene derivative - this work was done by dr. hab. J. Wojtkiewicz.

Experimental part is divided into three sections. The first one focuses on properties of donor polymers. Their optical absorption, luminescence and ESR and LESR spectra are provided. The second part is dedicated to CT process occurring at donor/acceptor interface. Therefore, it consists of results for blends of polymer and fullerene derivative. The CT process was characterized using two independent techniques - TRPL and LESR. In the case of effective photo-induced CT, luminescence quenching of polymer-fullerene derivative blend is observed

as compared to the luminescence of separate components. On the other hand, the photo-induced CT generates free carriers – holes and electrons, which appear in a LESR spectrum as two lines, one from positive polaron in polymer, and the other one from negative polaron in fullerene derivative. In order to check the influence of CT process on solar cell efficiency, such devices were built for selected polymers and characterized by *I-V* and photocurrent measurements, which were recalculated for external quantum efficiency. In the third part of experimental results we show that our elaborated methodology for characterization of material used in polymer organic solar cells can be also applied to study materials for other types of photovoltaics, such as organometal halide perovskite.

At the end of this thesis discussion and summary are given.