Photo-induced Charge Transfer in Third Generation Solar Cells

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The third generation solar cells (TGSCs) are considered as promising, cost-effective way to harness solar energy. They are built of semiconducting organic macromolecules, inorganic nanoparticles or hybrids.

We will present results of our studies of two sub categories of TGSCs, one based on polymeric donor and fullerene derivative acceptor, and the second one built from recently discovered hybrid perovskites.

In TGSCs the most important process deciding on efficient performance of solar cell is charge transfer (CT) occurring at the interfaces of TGSC components, after sun-light induced creation of excitons and their diffusion. An exciton dissociation is possible only with energy gain larger than the exciton binding energy. In the simplest picture, when neglecting Coulomb and exchange interactions within exciton pair and relaxation of atoms within molecules, the CT process is possible if HOMO (the highest occupied molecular orbital) and LUMO (the lowest unoccupied molecular orbital) levels have lower energies for an acceptor constituent than the respective energies for a donor constituent.

Two experimental techniques applied by us enabled observation of the CT process, namely Time-Resolved Photoluminescence (TRPL) and Light-Induced Electron Spin Resonance (LESR) Spectroscopies. In the case of effective photo-induced CT, luminescence quenching of donor-acceptor blend is observed as compared to the luminescence of separate components. On the other hand, the photo-induced CT generates free charges – holes and electrons, which appear in a LESR spectrum as two lines, one from positive polaron on a donor site, and the other one from negative polaron on an acceptor site.

Photo-induced CT process was studied in mixtures made of strong electron acceptor - [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) and polymers from polyazomethine group. As reference, we used results obtained by us for poly(3-heksylotiophene):PCBM blend, typically applied as donor-acceptor in bulk heterojunction polymer solar cells. Moreover, we studied CT process in $CH_3NH_3PbI_{3-x}Cl_x$ perovskite. For all the respective solar cells I-V characteristics were made, and also external quantum efficiency spectra were obtained.

From the TRPL and LESR experiments we determined polymer-fullerene blends having efficient CT and the ones, which performed not well. These observations were consistent with the respective solar cell efficiencies.

The experimental results were supported by our theoretical calculations of HOMO and LUMO energy levels, using the density functional theory method. These calculations allowed to determine what chemical modification of polyazomethines leads to change of their HOMO/LUMO energy levels and energy gap.

The full coherent picture of the studied solar cells consisting of (i) component material properties, (ii) corresponding solar cell efficiencies, and (iii) HOMO/LUMO model, will be presented.