ABSTRACT

Dissertation presents results of the research touching various aspects of organic photocells work. There are three major kinds of this explorations. First one focuses on BHJ architecture constraints. The second one embrances DFT computations for molecules of compounds obtained within POF and TechMatStrateg projects as the builders of the active layer in the organic solar cells. Finally, the third kind of explorations is formed by DFT computations carried out for the carbon nanotubes with the aim of identifyig possibilities of nanotubes applications in the organic solar cells.

Within the first group of problems, possibilities of improvement of the organic cells efficiency built in BHJ architecture (Bulk Heterojunction: the active layer consists of the randomly deployed nanoseeds of donor and acceptor) was investigated. That efficiency is far from the theoretical maximum. The suggestion that efficiency could be improved by making the cells in so called brush architecture was put forward. In order to investigate that a computer model of organic solar cells in the BHJ architecture was made. That model gives better understanding of the scale of the efficiency constraints in the BHJ architecture, as the consequence of the lack of arrangement in the active layer structure. They leads to the conclusion that the chaotic mixing of the donor and the acceptor materials does not cause the significant efficiency loss and for that reason an effort to obtain more organised structure will not bring wanted efficiency increase. The reason of unsatisfying organic solar cells efficiency must be seek elsewhere.

Within the secound group of problems the DFT calculations for the chemical compounds which potencially could be used to the organic solar cells processing were described. Calculatins were lead within POF and TechMatStrateg research programs. For usefulness as the electrons donors the polimers from the poliazomethines family were tested. On the other hand, as the potential electrons acceptors some fullerens derivatives were considered. Research was lead with the accessible software, deployed in quantum chemistry (Gaussian 09).

The third group of research is an amplification of idea to use the carbon nanotubes in the organic solar cells processing in the layer architecture. That concept is based on described in literature observations suggestive the exceptionally long exciton's diffusion way in the carbon nanotubes (order of 200 nm). Some problem could be here the carbon nanotubes absorption spectrum, which for various kinds of them consists usually of narrow bands, not covering the visible light scope. Theoretical possibility for composing the various kinds of carbon nanotubes mix with aggregated spectrum covering whole the visible light scope were examined then. Also that research had form of the theoretical computations with the quantum chemistry dedicated software.