EPR Studies of Functionalized C60 Fullerenes for Possible Applications in Photovoltaics

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The active layer of the most popular organic cell consists of two main components: donor polymer material – P3HT (poly(3-hexylthiophene-2-5-diyl)) and acceptor material – PCBM (phenyl-C61-butyric acid methyl ester). The basis for the operation of the solar cell is photo-creation of electron-hole pair in P3HT and further separation of electron and hole. The electron is transferred to fullerene while the hole stays in P3HT. The final efficiency of the solar cell is directly proportional to the effectivity of the aforementioned charge separation process. Currently, scientists are putting a lot of effort into further improvement of the active layer materials in order to achieve cells that are more efficient and easier to produce. Here we present studies of C60 fullerenes functionalized with tiophene or pyrene (Fig. 1) that enable separation of charges within one structure. This could be the first step to construct a single component active layer. EPR technique enables to extract signals from unpaired electrons and holes and thus is a suitable tool in studies of the effectiveness of charge separation in solar cells. In case of standard P3HT:PCBM active layer spectrum consists of two lines: one of g-factor equal to 2.002 corresponding to hole localized on P3HT and one of g-factor equal to 2.000 corresponding to electron localized on fullerene. In case of our functionalized fullerenes after illumination similar two distinct lines are present in the spectrum (Fig. 1) showing that charge separation process takes place, even in the absence of the donor polymer material in the system. The intensity ratio of the signal measured before and after illumination varies for each material. This allows us to determine the most efficient material. Additionally, the temperature and power dependencies of signal allow to extract spin relaxation time for each material. Materials with the highest charge separation potential will be considered for solar cell fabrication, in progress now.

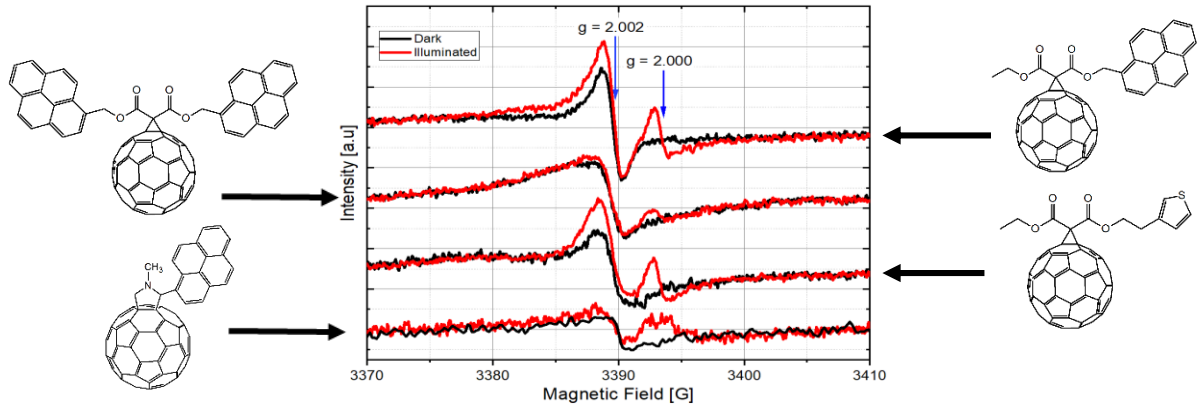

Fig 1. EPR spectra of C60 fullerene differently functionalized with pyrene and thiophene measured at 2K temperature. After illumination charge separation is manifested in observation of two distinct EPR lines: one corresponding to g-factor equal to 2.002 and the second corresponding to g-factor equal to 2.000.

Acknowledgment: Research was co-founded by project TECHMATSTRATEG1/347431/14/NCBR/2018 (National Centre for Research and Development).