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Interface structure of P3HT/SWNT blend and charge separation process on it KATSUHIKO NISHIMRA, RYOTA JONO, MIKIYA FUJII, KOICHI YAMASHITA, Department of Chemical System Engineering, University of Tokyo and JST, CREST — We investigated the mechanism that suppression of charge recombinations takes place in blends of regioregular Poly-3-HexylThiophene (rrP3HT) and semiconducting Single Walled Carbon Nanotube (scSWNT) only if excess P3HT exists. The rrP3HT/scSWNT blend seems to be suitable for OPV application because rrP3HT is common acceptor material and also can be used for purifying scSWNT and removing metallic one. Then the suppression of charge recombinations is attributed to unique helical supramolecular structure at P3HT/SWNT interfaces.[1] However, the detailed mechanism of the suppression has not been clarified yet. In this presentation, we show that side chains of P3HT are important in formation of the helical structure rather than alignment of main chains with graphene lattices of SWNT by using semi-empirical quantum chemistry method. Moreover, HOMO levels of P3HT molecules at the interfaces estimated to be lower than those in crystalline domain because of disordered stacking due to formation of the helical structure. This difference in HOMO levels can act as the driving force for escape of charge carriers from the interfaces and can result to the suppression of charge recombinations.

[1]S. D. Stranks et. al., **Nano. Lett.** 11, 66

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