Short-range conductivity in P3HT films doped by p-type F4TCNQ dopant.

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Doped conjugated polymers have high electrical conductivity due to charge carrier formation and thus understanding their transport properties is a key for their intelligent optimization and efficient application in organic electronics. Molecular p-doping of the poly(3hexylthiophene) (P3HT) with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) is a widely studied model system for this purpose.

However, the short-range conductivity over distances of few nm measured via time-domain THz spectroscopy (TD-THz) has never been investigated for this system. These measurements can reveal fundamental insights into the nature of short-range mobility and charge carrier density in p-type doped P3HT.

In this work, we study the THz conductivity of doped regioregular (RR) P3HT/F4TCNQ blends at various dopant concentrations (1-17 mol%) using solution processing method. Also, we used different regioregularities of P3HT –RR-P3HT (84%) and regiorandom RRa-P3HT (50%) - and show that they display different THz mobility. The charge carriers in the RRa-P3HT matrix are less mobile than in the RR-P3HT when doped with the same dopant concentration (9 mol%), due to disruption of the extended π-system that eventually lowers the effective conductivity. This information is obtained from Drude-Smith analysis on the THz spectroscopy data. We revealed that the short-range mobility and effective conductivity in P3HT/F4TCNQ blend films are sensitive to the regioregularity of polymer matrix, but not to the morphology of the doped films, which is found to be significantly affected and gradually disordered as the dopant concentration in the film increases. Also, doping concentration is found to affect the localization of the charge carriers. For doped RR-P3HT at lower doping concentrations (1-6 mol%) charges are more localized compared to higher doping regime (9-17 mol%) and this strongly impacts the effective THz mobility. Moreover, we show that simultaneous co-existence of integer charge transfer (ICT) and charge transfer complex (CTC) is observed in high doping ratios (13 mol% and 17 mol% blends of RR-P3HT/F4TCNQ and 9 mol% blend of RRa-P3HT/F4TCNQ), that support that doping mechanisms depend on the degree of regioregularity of host polymer and dopant concentration. Based on the obtained results, we believe that both bound and free charge carriers have contribution on short-range conductivity, however, more deep and detailed analysis should be done to better understand the interplay between ICT and CTC doping mechanisms.

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