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Monte Carlo modeling of the spatially dispersive carrier transport in P3HT and P3HT:PCBM blends XIN JIANG — The presence of traps, arising from morpohological or chemical defects, can be critical to the performance of organic semiconductor devices. Traps can reduce the charge carrier mobility, disturb the internal electrical field, drive recombination, and reduce the overall device efficiency as well as operational stability. In this work, we investigate the role of traps in determining charge transport properties of organic semiconductors and blends such as P3HT and P3HT:PCBM through Monte-Carlo (MC) simulations in conjunction with time-of-flight (TOF) mobility measurements. We employ a Marcus theory description of individual hopping events based on the molecular reorganization energy (lambda) for the MC simulations. Trap states are modeled as diffuse bands that reside at some energy away from the main transport band. This model is used to simulate TOF transients, and the results are compared to experimental data. As is expected from the Marcus theory equation, the mobility is seen to be maximum for an optimal value of lambda. This optimal value is strongly field dependent, but is found to be independent of the trap density. In comparing MC simulations with TOF data, it is found that inclusion of traps results in a much better fit to the data and provides for a mechanism to simulate dispersive transport with a long tail resulting from trapping and detrapping of carriers before they exit the device. We present results for a range of trap densities and statistical distributions and discuss the implications on the operation of bulk heterojunction organic photovoltaic devices.

Xin Jiang

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