Electron Kinetics in Disordered Organic Semiconductors

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A three-dimensional Kinetic Monte Carlo Simulator has been implemented to bridge the gap between molecular dynamics and ensemble Monte Carlo techniques in the field of organic microelectronics. By assigning an individual time scale to each single event a kinetic, rate-based description of the dynamics is enabled, which describes the system's evolution towards its steady state in a chronological sense. The simulations focus on the dispersive regime, where long-tailed waiting time distributions account for the fact that the time scales assigned may vary over several orders of magnitude. Since the charge flow in an organic device strongly depends on interfaces and boundaries, an Au/ZnPc/Au-device is simulated in-situ. In particular injection, propagation, and ejection of electrons obeying the Pauli-principle are treated by one single transition rate which also rules transitions between bonding and antibonding orbitals. Current-voltage characteristics for films up to a length of 140 nm have been simulated.