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Cooperative Electron-Hole Dynamics at the Organic Donor-Acceptor Interface[1] CHEE KONG LEE, SHI LIANG, ADAM WILLARD, Massachusetts Institute of Technology — Charge transfer (CT) excitons are Coulombically bound electron and hole pairs located in spatially separate regions. They play an important role in both light emission of organic light emitting devices and the generation of photocurrent in organic photovoltaic. For some donor/acceptor blends the lowest electronic excitations are triplet CT states, and in these materials the photoluminescence and photocurrent generation exhibit a non-trivial magnetic field dependence due to its effect on singlet-triplet intersystem crossing and reverse intersystem crossing rates. Recent experiments have demonstrated that in these materials bound electron-hole pairs can move geminately over distance of 5-10nm confirming the transport of CT excitons despite strong Coulombic attraction. These experiments can be understood with a numerical model combining kinetic Monte Carlo and the quantum master equation. The model contains a minimal set of physical elements, and yet is able to quantitatively reproduce the experimental results. More importantly, the model provides insights into properties that otherwise cannot be obtained from experiments. Here I present the details of this model along with the physical insights it has provided into this particular class of materials.

[1]Cooperative Electron-Hole Dynamics at the Organic Donor-Acceptor Interface

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