Energy Disorder and Device Performance in Organic Electronics

C.F. Madigan, V. Bulović
Sponsorship: MARCO MSD, NDSEG Fellowship

Presently many organic electronic devices employ amorphous materials, and it is well known that the molecular energy levels in such materials are subject to disorder arising from variations in local intermolecular interactions. The movement of molecular charge carriers and excitons through the constituent materials largely controls the performance of such devices, and it has been well established that energy disorder strongly influences charge carrier and exciton motion. Though accurate analytic treatments remain elusive, Monte Carlo (MC) simulations of charge carrier and exciton hopping between molecular sites subject to energy disorder have proven an effective tool for analyzing charge carrier and exciton motion in such materials [1]. Combining MC simulations with accurate models of energy disorder should make it possible to perform calculations of device behavior in realistic structures with relatively few theoretical model assumptions. This project addresses: (1) the theoretical calculation of energy disorder in amorphous organic materials; and (2) the application of MC simulations to realistic device structures and operating conditions. We have performed exact calculations of charge carrier and exciton energy disorder arising from electrostatic interactions between structurally disordered, polarizable molecular charge distributions (see Figure 1). These calculations differ from those in the literature because the molecular polarizibility is explicitly included in the calculation, avoiding the need to employ dielectric continuum approximations (DCAs). It is found that the widely used DCAs are inaccurate, and we presently are developing improved expressions for relating the magnitude of the disorder to the material properties (principally, the molecular dipole moment, the molecular density, and the dielectric constant). We have also developed an MC simulator of charge carrier and exciton motion in energetically disordered molecular materials capable of treating realistic device geometries (e.g., multilayer stacks and electrical contacts). Because organic electronic devices often operate at high carrier concentrations, we have also included basic charge-carrier interactions to treat the effects of carrier concentration on charge transport; these effects have not been previously investigated using the MC simulation technique. We are presently performing calculations of carrier mobilities as a function of field and carrier concentration (see Figure 2) for comparison with existing approximate analytic approaches. These studies support future simulations of real device structures for a rigorous comparison of experimental device performance and theory.

**REFERENCES**