Public Abstract

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Title:Raman scattering studies and charge transport in polyfluorenes.

Conjugated polymers (CPs) are an important class of organic semiconductor that finds application as electronic materials in a range of low cost consumer electronics. Recently one particular class of CP, polyfluorene (PF), a prototypical fluorene-based homo polymer has received a lot of attention due to its high luminescence efficiency and excellent electronic properties which provides great prospect for device applications. The performance of devices based on these polymers depends on side chain conformations, overall crystalline structure, and charge transport processes at the microscopic level. This project entails detailed Raman scattering studies and charge transport properties of two side chain substituted PFs: Poly(2,7-[9,9'-bis(2-ethylhexyl)] fluorene) (PF2/6) and Poly(9,9-(di-n,n-octyl) fluorene) (PF8). The structural properties of PFs are extremely sensitive to the choice of functionalizing side chains, PF8 adopts metastable structures that depend upon the thermal history and choice of solvents used in film forming conditions. Raman scattering is an important spectroscopic technique to characterize the structure, electronic excitation, and morphology of different phases of this polymer at different temperatures. Raman scattering techniques as a function of thermal cycling are used to monitor the changes in the backbone and side chain morphology of PF8. These studies establish a correlation between the conformational isomers and the side and main chain morphology. Electroluminescence and photoluminescence measurements from PF-based light-emitting diodes (LEDs) are also presented and discussed in terms of the crystalline phases and chain morphologies in the PFs.

The charge transport properties of PF-based CP critically depends on efficient charge carrier injection, the degree of ordering of the chains, their crystalline structure in the solid state as well as density of chemical and/or structural defects (traps) which lies at the metal organic interfaces as well as in the bulk. In this research work charge carrier injection and transport properties of PF-based LEDs are presented using current-voltage characteristic which is modeled by a space-charge-limited conduction (SCLC) for discrete and continuous traps. PF2/6 with a high level of molecular disorder is an exemplary system for the SCLC model with discrete single level shallow traps. Charge transport as a function of sample thickness uncovers the origin of these traps. Temperature dependence of and dc conductivity measurements suggest thermal assisted variable-range hopping transport instead of band transport in these materials.

Charge carrier injection and doping in CPs induce structural deformation with the formation of self-localized excitation states, such as polarons or bipolarons inside the band gap. Raman scattering studies of PF2/6-based LEDs with doping and in the presence of injected and photo-generated charge carriers show increasing backgrounds with asymmetric Briet-Wigner Fano (BWF) line shapes, indicating strong electron-phonon interactions.