

Public Abstract

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Title:HIGH PRESURE SPECTROSCOPIC STUDIES OF ORGANIC DEVICE MATERIALS

The optical and electronic properties of organic semiconductors (di-octyl substituted polyfluorene, ladder type poly(para-phenylene) (LPPP) and donor-acceptor polymer heterojunctions) are investigated under high pressure. A comparison of the photoluminescence spectra of as-is and thermally cycled di-octyl substituted polyfluorene (PF8) under pressure is found to be an ideal tool for identifying the different ingredients that impact the shift of the optical energy gap. Our observations have disentangled inter- and intra-chain interactions. The Raman study shows a strong electron-phonon interaction between the Raman phonon and the electronic continuum. Photoluminescence and phosphorescence studies of PhLPPP show evidence, for the first time, that the singlet-triplet energy splitting remains almost a constant under enhanced intermolecular interaction. These findings provide an insight into the effect of inter- and intramolecular interaction in the organic device materials, which might lead in the development of more efficient organic LEDs and field effect transistors.

Bulkheterojunction polymer solar cells are based on a composite blend of two materials with electron donating and electron accepting properties. For the bulkheterojunctions of P3HT or PhLPPP with PCBM, study of the photoluminescence and absorption spectra under pressure reveal that the LUMO band-edge offset increases with pressure. Vibrational studies of pristine P3HT and P3HT:PCBM blend show that the molecular ordering is barely affected by pressure in the pristine P3HT, whereas the ordering decreases with pressure in PCBM blended P3HT beyond 3.0 GPa. These findings provide a platform for theoretical modeling of a very promising set of organic solar cell materials for enhanced device performance and functionality.