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Molecular Dynamics of F8BT Polymer Film: Correlation with Opto-Electronic Properties

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Poly(9,9'-dioctylfluorene-*co*-benzothiadiazole) (F8BT) is currently one of the most promising material for use as active layers in polymeric electronic devices, such as polymer light-emitting diodes (PLEDs) and polymer field effect transistor (P-FET). It is well known that both polymer structure and dynamics affects either the luminescence or transport properties in thin films, making worthwhile to investigate them. Dynamical aspects of F8BT were first investigated by Dynamical Mechanical Thermal Analysis (DMTA), Differential Scanning Calorimetry (DSC) and ¹H Nuclear Magnetic Resonance (NMR). The results revealed the presence of two main relaxation process, which occurs at about 225 K (β -relaxation) and 370 K (α -relaxation). The molecular processes responsible by such relaxations were investigated by specific NMR experiments, such as Dipolar Chemical Shift correlation (DIPSHIFT) and Centerband Only Detection of Exchange (CODEX). The results showed that, in the temperature range of 220 to 373 K, the lateral chain execute molecular rotations with average correlation times ranging from 10^{-4} – 10^{-7} seconds. On the other hand, from 300 to 350K the backbone carbons execute slow libration motions with reorientation angles that increase as a function of temperature. Those results could be correlated with the Current-Voltage characteristics of thick ITO/F8BT/Al devices carried out a several temperature (70 until 490 K). The drift charge mobility in the device was studied as a function of temperature by Time of Flight techniques (TOF), showing relatively abrupt change on the activation energy near both relaxations (β and α). Based on these results, a model that explains the behavior of the charge transport as a function of temperature based on the occurrence of the molecular relaxation was proposed.