How can the Nanostructure Affect the Charge Transport in PLED?

M.M.D. Ramos[a], H.M.C. Barbosa[b]
Department of Physics, University of Minho, Campus de Gualtar, 4710-057, Portugal
[a]marta@fisica.uminho.pt, [b]helder@fisica.uminho.pt

Abstract
Modelling the functioning of organic optoelectronic devices that uses polymers as one of the components is a difficult task since most of the polymers present a complex nanostructure. In the active layer, depending on the experimental conditions used to deposit the polymer, the polymer chains can be placed between the electrodes forming domains with different orientations relative to the electrodes surface and this can influence the device performance. Theoretical studies have shown that when a charge is injected into a polymer strand, it can moves along the polymer strand (intramolecular mobility) depending on the orientation of the strand relative to the local electric field, and this will affect charge bulk mobility. Although it is known that in real polymer light emitting devices charge transport is influenced by many factors like the presence of chemical charge traps, physical defects, etc, that can mask the influence of the nanostructure and the polymer intramolecular properties in charge transport, in pristine polymer layers these effects can be more notorious. Therefore, we performed computational experiments to understand the effect of the nanostructure (e.g. polymer strand orientation) in the performance of polymer light emitting diodes (PLEDs) using a generalized dynamical Monte Carlo method. Our results show that in pristine PLEDs the electric behaviour has a dependence on the polymer nanostructure and this is related to the contribution of intramolecular charge mobility to the overall charge transport in the device.