

MAR15-2014-003490

Abstract for an Invited Paper  
for the MAR15 Meeting of  
the American Physical Society

**Percolation, tie-lines, and the microstructural determinants of charge transport in semicrystalline conjugated polymers**

ANDREW SPAKOWITZ, Stanford University

Semiconducting polymers play an important role in a wide range of optical and electronic material applications. It is widely accepted that the polymer ordering impacts charge transport in such devices. However, the connection between molecular ordering and device performance is difficult to predict due to the current need for a mathematical theory of the physics that dictates charge transport in semiconducting polymers. Here, we present a new analytical and computational description in which the morphology of individual polymer chains is dictated by well-known statistical models and the electronic coupling between units is determined using Marcus theory. This effort combines our research group's modeling efforts in polymer conformational properties and reaction-diffusion phenomena to address the multiscale dynamics of charge transport in a heterogeneous material. The resulting model is capable of bridging molecular-level charge transport mechanisms to large scale transport behavior, thus facilitating direct comparison with experiments. The multiscale transport of charges in these materials (high mobility at short length scales, low mobility at long length scales) is naturally described with our framework. Additionally, the dependence of mobility with electric field and temperature is explained in terms of conformational variability and spatial correlation. Our model offers a predictive approach to connecting processing conditions with transport behavior.