

Charge Transport and Molecular Order in Semiconducting Polymers

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Organic thin film electronic devices are attractive due to their low cost of fabrication. The optoelectronic properties of semiconducting polymers have long been studied for applications in conductors, light emitting diodes, solar cells, and thin film transistors (TFTs). Despite the significant progress in the development of high performance devices, it is still difficult to connect the molecular scale features of these materials with transport over long range length scales.

We will present recent work on developing a better understanding of the connection between molecular order and charge transport. First we will discuss how the correlation length of the backbone of semiconducting polymers is related to charge carrier mobility in thin film transistors. Second we will discuss how molecular ordering can be used to design thermally stable electrically doped polymer films.

Short range crystalline molecular order is known to lead to high carrier mobility in polymer TFTs although such ordering is known not to be essential in all cases. We have used a novel small angle soft x-ray scattering method to reveal long range ordering in films of poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-*b*]thiophene), PBTTT as a function of processing conditions. We find that long range order is highly correlated with the field effect mobility in TFTs formed with polymer dielectrics while short range crystalline order is not. These results are consistent with models of charge transport suggesting that alignment of ordered domains leads to higher mobility.

Controlling the electrical conductivity of semiconducting polymer is difficult despite its relevance to controlling charge injection and the Fermi level in organic devices. We have studied how molecular dopants can be used to dope both *p*- and *n*-type polymers and find that molecular interactions can be used to rationalize the thermal stability of the electrically doped films. For example, relatively low concentration doping by the acceptor, F4TCNQ, causes both increased electrical conductivity in PBTTT and substantial structural changes including a decrease in the π -stacking distance between ordered polymer chains. These significant changes in intermolecular ordering upon carrier formation that must be addressed in models of charge transport.