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Electronic states at the interface between crystalline and amorphous domains in conjugated polymers

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Abstract. Materials based on conjugated polymers exhibit complex structure with interlaced crystalline and amorphous domains [1]. In this work, microscopic insight into the electronic states at the interface between amorphous and crystalline domains in poly(3-hexylthiophene) (P3HT) is given for the first time. We have considered two types of the interface: (1) sharp interface, where polymer chains belong to ideal crystalline or amorphous domain (type A) and (2) interface that consists of extended chains, where chains are extended out from crystalline domain and have the end in amorphous domain (type B). Type B interface is generally believed to be more representative of interfaces that occur in real interfaces. Atomic structures were generated using Monte Carlo simulations, while electronic structures were calculated using density functional theory-based charge patching method [2] and overlapping fragments method [3]. Results show that wave functions of highest states in the valence band are delocalized and belong to the crystalline domain (Fig. 1a), regardless of the interface type. On the other hand, highest states in amorphous regions are localized on one or two chains (Fig. 1b). In the case of type A interface, we also find the states localized at the interface with the energy between the band edge energies of the crystalline and amorphous region. HOMO offset in the case of type B interface is around 0.5 eV, while in the case of type A interface it is even larger. These offsets present high barriers for holes, which implies that hole transport dominantly goes across crystalline regions.

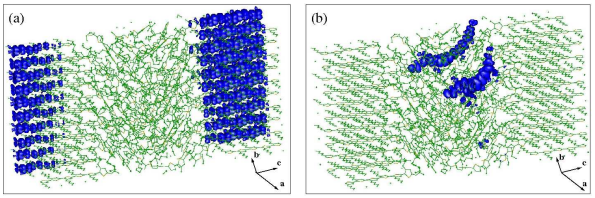

FIGURE 1. Wave function moduli of the (a) highest electronic state in the valence band in the crystalline domain and (b) highest electronic state in the valence band in the amorphous domain in the case of type B interface.

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