Electronic Properties of Interfaces between Domains in Organic Semiconductors

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The aim of this thesis is to provide a link between atomic and electronic structure of different types of interfaces between domains in organic semiconductors. In polycrystalline small-molecule organic semiconductors interfaces are formed between single crystalline domains. We found that grain boundaries in polycrystalline naphthalene introduce trap states within the band gap of the material [1,2]. Trap states are localized on closely spaced pairs of molecules from opposite sides of the boundary. Realistic conjugated polymers, such as poly(3-hexylthiophene) (P3HT), contain mixed crystalline and amorphous domains. We found that HOMO state of the interface between crystalline and amorphous domain in P3HT belongs to crystalline domains [3]. States that belong to both domains and trap states were not found. Effects of thermal disorder are important in realistic conjugated polymers. Our results show that disorder in backbone chains of P3HT has strong effect on the electronic structure and leads to the localization of the wave functions of the highest states in the valence band, similar to the ones that occur in amorphous polymers [2,4]. At the interfaces between two materials in organic electronic devices, effects of spontaneous polarization in one or both of them on electronic properties can be pronounced. We show that ordered P3HT exhibits spontaneous polarization along the backbone direction, which is caused by the lack of inversion symmetry due to head-to-tail side chains arrangement [5]. We additionally show that spontaneous polarization in ordered P3HT keeps significant values even at room temperature when the effects of thermal disorder are important.

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