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Atomistic Molecular Dynamics Simulation of the Surface Properties of P3HT Films[1] YENENEH YIMER, SIMA MOFAKHAM, ALI DHINOJWALA, MESFIN TSIGE, Department of Polymer Science, University of Akron — In recent years P3HT has attracted much interest mainly because of its potential applications in solar cells, light emitting diodes and field effect transistors. The performance of these devices is strongly dependent on the structural packing, morphology and interfacial properties of the P3HT. In order to improve the devices efficiency, understanding the structural and dynamical properties of P3HT at the atomic level is important. Most studies on P3HT have mainly focused on understanding its bulk properties. However, the orientation of P3HT chains at the polymer/air interface has not been well investigated. Using molecular dynamics simulations we have studied the interfacial properties of free-standing P3HT films. The simulation results show that at the air/polymer interface the alkane side groups of the P3HT chains orient mainly to the interface in qualitatively good agreement with SFG experimental results. The surface tension of P3HT in its melt state shows strong dependence on temperature and chain length and is directly related to the roughness of the P3HT surface.

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