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Structural and Morphological Analysis of Poly(3-hexylthiophene) at Surfaces and Interfaces[1] YENENEH YIMER, MESFIN TSIGE, Department of Polymer Science, The University of Akron — The structure and morphology of semiconducting polymers such as Poly(3-hexylthiophene) (P3HT) at surfaces and interfaces have significant influence over the performance of organic solar cell devices. Because charge-carrier generation, transport to and collection at the electrodes depend on the material properties of P3HT - themselves controlled by factors including packing, orientation and environment - analysis of the mechanisms that contribute to efficient charge generation and minimization of recombination is necessary. Using molecular dynamics simulation, we have investigated the structural properties and morphological evolution of P3HT at different surfaces and interfaces. We have also investigated the dependence of those properties on temperature, chain length, and interfacial energies. The morphology of P3HT is correlated to efficient charge transport. Using our analyses, we have attempted to elucidate these correlations, which should help lead to optimization of the morphology of P3HT in devices in the pursuit of increasing the efficiency of polymeric devices.

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