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Molecular Ordering of Poly(3-hexylthiophene) on Self-Assembled Monolayers[1] YENENEH YIMER, MESFIN TSIGE, Department of Polymer Sceince, The University of Akron — The molecular ordering of semiconducting polymers such as Poly(3-hexylthiophene) (P3HT) at surfaces and interfaces has significant influence on the performance of organic solar cell devices. The charge-carrier transport and the charge collection at the electrodes strongly depend on the molecular ordering of P3HT at interfaces. Molecular ordering of P3HT can be tuned by varying the substrate surface chemistry and film processing conditions. Using all-atom molecular dynamics simulations and validated force field parameters, we have investigated the molecular ordering of P3HT on self-assembled monolayers (SAMs) of n-alkanethiols with varying end-functional groups and spacer length. In this study we elucidate the dependence of the molecular ordering of P3HT (edge-on or face-on conformation) on the surface chemistry of SAMs. Moreover, we investigated the effect of solvent on the molecular ordering of P3HT on SAMs surfaces. Understanding the correlation between P3HT morphology and surface chemistry will help in designing P3HT-based solar devices with better efficiency.

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