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**Oligothiophene/fullerene interfaces: Molecular Simulations of Organic Photovoltaic Materials** SRIDHAR YERUSU, Graduate student, Department of Chemical and Materials Engineering, University of Cincinnati, VIKRAM KUPPA, Assistant Professor, Department of Chemical and Materials Engineering, University of Cincinnati — Atomistically detailed molecular dynamics simulations are used to study the interface between quaterthiophene and fullerene, prototypical molecules in organic bulk heterojunction solar cells. The simulation mimics the morphology that provides optimized generation of free charges from photogenerated excitons in such assemblies, as studied by experiment. The effect of temperature and the presence of a rigid fullerene phase on the behavior of the conjugated polymers are explored. Order parameters of chain orientation demonstrate that significant fractions of the oligothiophene molecules align along directions of the form <110>, parallel and adjacent to the C60 substrate. It is seen that the surface influences the stacking of thiophene rings, which is crucial to facilitating effective charge transport in organic semiconductors, due to the resulting overlap of $\pi$-electron clouds. The distribution of ring orientations reveals the relative stacking of rings as a function of the distance from the fullerene phase. The simulations also investigate the dynamics of backbone dihedral libration in the oligothiophenes. Our goal in performing these simulations is to provide fundamental insights into the mechanisms that govern the overall efficiency of polymeric optoelectronic devices.

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