Solar cells constructed from organic materials have emerged in recent years as a potentially viable technology for renewable energy. Organic photovoltaic (OPV) devices are especially appealing due to the potentially low cost of their materials and production in comparison to their inorganic counterparts. However, the relatively low power conversion efficiency of OPV devices has hampered their widespread adoption. Organic photovoltaic devices are typically fabricated from two active components: a light absorbing polymer and a fullerene derivative which aids exciton dissociation and electron transport. However, typical fabrication techniques for OPV devices do not allow for precise control of the devices’ structural morphology. The effects of this internal structure on device performance and behavior are not yet fully understood and remain an area of active research. In order to elucidate the effects of the internal morphology on OPV device performance, we have developed device modeling capabilities based on the classical Drift-Diffusion model. Our studies have illustrated the profound effects that the distribution of components within the active layer of an OPV device may have on its resulting device physics. Furthermore, our modeling capabilities allow us easy access to data that is not experimentally trivial to obtain, such as charge carrier densities and recombination rates. With these capabilities, we have shown how vertical phase segregation of conducting material away from an extraction electrode may result in exceptionally low-performing solar cells possessing an S-shaped J-V characteristic. We also illustrate how the structural disorder of an OPV morphology can inhibit device performance via a 1-D ensemble averaging technique. Finally, we present full 2-D simulations of OPV morphologies that illustrate the role in charge transport of the intermixed region between pure domains of polymer and fullerene that exist in typical OPV devices.

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