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Multi-scale Modeling Study of poly(3-hexylthiophene) and [6,6]-phenyl-C_{61}-butyric acid methyl ester Towards Organic Photovoltaic Cell Application HANJONG YOO, KI CHUL KIM, SEUNG SOON JANG, Georgia Inst of Tech — To date, organic photovoltaic cells have gained attention due to their promising potential in the industry. Its efficiency needs to be improved through constructing better morphologies. There are three morphological quantities that affect the efficiency. The domain size of the electron donor phase has to be small and the interface-to-volume ratio of the blend must be large. The percolation ratio has to be high. To investigate the morphological properties of the active layer systems, the state-of-the-art multi-scale modeling is employed. In this study, P3HT and PCBM blends have used as our active layer candidates. We have developed our own force field parameters to accurately describe potential energy surfaces in the layer systems. Subsequently, coarse-grained force field for P3HT and PCBM have been developed based on the improved atomistic force field parameters in order to simulate larger systems. The results from coarse-grained models are validated through the comparison with those from the full atomistic models. Using the molecular dynamics simulations, the newly developed coarse-grained models will be further used to study how the crystallinity of P3HT affects the morphological properties in the active layers.

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