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**Active layer morphologies for device simulations** JUTTA LUETTNER-STRATHMANN, KIRAN KHANAL, Departments of Physics and Chemistry, The University of Akron — The morphology of the active layer has a strong effect on charge generation and transport in organic photovoltaics. In bulk heterojunction devices, amorphous and crystalline regions with varying compositions coexist due to microphase separation and crystallization of the blend components. Accounting for these effects in device simulations is difficult since the size of the active layer is too large to generate realistic morphologies from molecular simulations of the constituents. In this work we perform Monte Carlo simulations of a coarse-grained lattice model of polymer mixtures to generate microphase separated layers with ordered and disordered regions. We employ external fields and surface interactions to control the morphologies and investigate the effect of domain size and distribution on charge transport.

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