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Effect of Structure on Charge Mobility in Partially Ordered Polymeric Systems WAYLON LUO, KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, University of Akron — The performance of thin film organic semiconductor devices depends on the mobility of the charge carriers, which is strongly affected by the structure of the material. 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 present Monte Carlo simulations of a coarse-grained lattice model for dense polymeric systems with a semiflexible component that undergoes a transition to (partially) ordered states at low temperatures. To investigate charge transport, the lattice polymer configurations become part of a model device, which consists of a layer of the material between two electrodes at different potentials. We determine the mobility from Monte Carlo simulations of charge carriers. To model the effect of polymer chain connectivity on charge transport we include an energetic barrier to hopping between sites on different chains; energetic disorder is taken into account by averaging over many polymer configurations. We find that ordering in the material leads to strong mobility anisotropies with increased mobility for transport parallel to the ordered domains and reduced mobility for perpendicular transport.

Jutta Luettmer-Strathmann
University of Akron

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