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A Semi-Empirical Multi-Scale Dynamic Monte Carlo Model of Organic Photovoltaic Performance in RIR-MAPLE Bulk Heterojunction Films ADRIENNE STIFF-ROBERTS, AYOMIDE ATEWOLOGUN, Duke University (RT-MRSEC) — A semi-empirical method for investigating the performance of OPVs in resonant infrared, matrix-assisted pulsed laser evaporation (RIR-MAPLE) films is explored. Emulsion-based RIR-MAPLE offers a unique experimental backdrop for investigating trends through simulation and gaining a better understanding of how different thin film characteristics impact OPV device performance. A novel multi-scale formulation of the Dynamic Monte Carlo (DMC) model is developed based on observable morphology features. Specifically, using confocal microscopy, we observe the presence of micro-scale regimes of pure materials and nano-scale regions of the composite blend. This enables us to assign weighted percentages to DMC implementations on two different scales: the microscale and nanoscale regions. In addition to this, we use input simulation parameters acquired by characterization of as-deposited films. The semi-empirical multi-scale model presented serves as a unique simulation opportunity for exploring different properties of RIR-MAPLE deposited OPVs, their effects on OPV performance and potential design routes for improving device efficiencies. This work was supported, in part, by the Office of Naval Research under Grant N00014-10-1-0481 and the NSF Triangle MRSEC on Soft Matter.

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