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A Dynamic Monte Carlo Model with an Improved Charge Injection Mechanism for the Photocurrent Generation of Organic Solar Cells DYLAN KIPP, VENKAT GANESAN, The University of Texas at Austin — Previous dynamic Monte Carlo studies have made great strides in connecting organic solar cell device microstructure to final properties. One challenge still remaining is to capture the full illuminated and dark current-voltage curves and their dependencies on the charge injection mechanism. By modifying the injection mechanism of previous algorithms, we have developed an improved model for the simulation of photocurrent generation in organic solar cells. We include and utilize an injection rate prefactor to control the portion of dark current attributed to each of 4 kinds of charge injection. By shifting the dark current between electrode-polymer pairs, the injection timescales are aligned even when modeling ohmic contacts. Using our model, we are able to generate charge density and potential profiles that better agree with theory and better reproduce experimental results as compared to previous dynamic Monte Carlo methods. We are able to demonstrate how charge accumulation and band bending effects the shape and placement of the various current-voltage regimes. Finally, we are able to demonstrate how various parameters influence the current-voltage characteristics.

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