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Dynamic Monte Carlo Modeling of Exciton Dissociation in Organic Donor-Acceptor Solar Cells MICHAEL HEIBER, ALI DHINOJWALA, University of Akron, Department of Polymer Science — A general dynamic Monte Carlo model for exciton dissociation at a donor-acceptor interface including exciton delocalization and hot geminate pair dissociation has been developed to model the experimental behavior observed for the P3HT:PCBM system and predict the theoretical performance of future materials systems. The presence of delocalized excitons and the direct formation of separated charge pairs has been recently measured by transient photo-induced absorption experiments, and has been proposed to facilitate charge separation efficiency. The excess energy of the exciton dissociation process has also been observed to have a strong correlation with the charge separation yield for a range of thiophene polymer:PCBM systems, suggesting that a hot charge separation process is also occurring. Hot geminate pair dissociation has been previously theorized as a cause for highly efficient charge separation, however a detailed model for this process has not been implemented and tested. Here, both conceptual models have been implemented into a dynamic Monte Carlo simulation and tested using a model bilayer donor-acceptor system.

Michael Heiber
University of Akron

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