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Introducing Correlations into Carrier Transport Simulations of Disordered Materials through Seeded Nucleation: Impact on Density of States, Carrier Mobility, and Carrier Statistics[1] JOSHUA BROWN, SEAN SHAHEEN, University of Colorado Boulder — Disorder in organic semiconductors has made it challenging to achieve performance gains, this is a result of the many competing and often nuanced mechanisms effecting charge transport. In this article, we attempt to illuminate one of these mechanisms in the hopes of aiding experimentalist in exceeding current performance thresholds. Using a heuristic exponential function, energetic correlation has been added to the Gaussian Disorder Model (GDM). The new model is grounded in the concept that energetic correlations can arise in materials without strong dipoles or dopants, but may be a result of an incomplete crystal formation process. The proposed correlation has been used to explain the exponential tail states observed in these materials. It is also better able to capture the carrier mobility field dependence when compared to the GDM. Investigation of simulated current transients shows that the exponential tail states do not necessitate Montrol and Scher fits. Furthermore, we observe that sites located at the boundaries between the seed sites experience the most energetic deviation, are the source of the extended exponential tail states, and are responsible for high charge visitation frequency which may ultimately be associated with material stability.

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