

effect on the device current density. This is because the main driving force for the last step of recombination is the exciton binding energy, which is much larger than the energetic disorder σ . This result is well reproduced by the “percolation-corrected nearest-neighbor” ME model proposed in this work (full curves in the figure). In contrast, using a “local” ME model would give rise to strongly deviating results (dashed curves).

D . CURRENT- VOLTAGE CHARACTERISTICS BELOW THE BUILT-IN VOLTAGE

To further investigate the validity of the bipolar 3D-ME simulation model, we examine the current density-voltage characteristics around and below the built-in voltage V_{bi} . In this regime, the current density is dominated by diffusion rather than drift. The current increases exponentially with voltage. KMC simulations are then not realistically applicable due to an impractically long simulation time (Figs. 1A-B). In this subsection, we study the dependence of the ideality factor η , which is defined as $\eta = [3/4T/e \cdot d(\ln J)/dV]^{-1}$, on the disorder energy, voltage and temperature. The 3D-ME simulation results are shown in Figs. 8 and 9.

The ideality factor, obtained from the slope of the current density-voltage characteristics, enters the generalized Einstein relation between the diffusivity D and the mobility μ , $D = \eta \mu k_B T / e$. For nondegenerate inorganic semiconductors, $\eta = 1$. For disordered organic semiconductors, with a Gaussian DOS, $\eta > 1$ when the DOS is filled above the critical concentration beyond which the system is not anymore in the independent-particle (Boltzmann) regime. The ideality factor η is a function of the disorder parameter σ and the carrier concentration c . In a device, the carrier concentration profile is not uniform. That implies that the ideality factor as deduced from experiments can depend on the voltage at which it has been determined, as will be shown below.

It is not straightforward to directly compare the simulated ideality factor with the experimentally measured ideality factor in literature. The difference might come from three reasons. (a) In our simulations we consider a Gaussian DOS, but in reality there might be a superimposed exponential trap DOS, which is not included in our model. The exponential trap DOS will significantly modify the ideality factor. (b) As the ideality factor is extracted from the slope of the current density-voltage