

the percolative motion of the charge carriers in the disordered material. In contrast, the denominator in Eq. (9) does not include the effects of percolation, and therefore overestimates the rate with which electron-hole encounter processes will occur. The mobility that would follow from a such a weighted summation of local hopping rates, termed the “mean medium approximation” (MMA), is for the case of nearest-neighbour hopping in a Gaussian DOS given by (see Sec. V):

$$\mu(c) \cong \frac{2\beta a^2 e \nu_1}{\sigma} \times f(\hat{\sigma}, c)_{\text{MMA}} \times \exp[-0.25 \hat{\sigma}^2], \quad (12)$$

with $\beta = 0.562$ and $f(\hat{\sigma}, c)_{\text{MMA}}$ a function that in the limit of strong disorder becomes equal to the charge carrier concentration enhancement of the mobility with respect to the mobility for small carrier concentrations (see Figs. 10 and 11). For small disorder parameters, $f(\hat{\sigma}, c)_{\text{MMA}}$ approaches $\hat{\sigma}/2\beta$, consistent with the expression for the mobility in the disorderless limit, given above. Based on these results, we include the effect of percolation in the expression for the recombination prefactor by generalizing Eq. (10) in the following manner:

$$\begin{aligned} \gamma &= \frac{e^2 r_\mu r_\nu}{3\varepsilon_r \varepsilon_0 a k_B T} \frac{\mu_{\text{EGDM}}}{\mu_{\text{MMA}}} \\ &= \frac{e^2 r_\mu r_\nu}{6\beta \varepsilon_r \varepsilon_0 a k_B T} \frac{f_{\text{EGDM}}}{f_{\text{MMA}}} \exp[-0.17 \hat{\sigma}^2]. \end{aligned} \quad (13)$$

This theoretical approach is expected to yield a useful parameterization scheme describing the disorder, temperature and carrier concentration dependence of the value of γ that leads to optimal agreement between 3D-ME and 3D-KMC results. Based on Eq. (13), we will write

$$\gamma \cong A_{\text{th}} \frac{e^2}{\varepsilon_r \varepsilon_0 a k_B T} \exp[-B_{\text{th}} \hat{\sigma}^2], \quad (14)$$

with from the theory developed above $A_{\text{th}} = r_\mu r_\nu /_{\text{EGDM}} / (6/3/\text{MMA})$ and $B_{\text{th}} \cong 0.17$. Both parameters are dimensionless.

In Fig. 2, the value of A_{th} as a function of the disorder parameter $\hat{\sigma}$ and the carrier concentration c is given (details of the evaluation are given in Fig. 12). Surprisingly, although $/_{\text{EGDM}}$, $/_{\text{MMA}}$, r_μ , and r_ν are all $\hat{\sigma}$ and c dependent, their combination A_{th} is only weakly sensitive to $\hat{\sigma}$ and c in the range $3 \leq \hat{\sigma} \leq 5$ and $10^{-6} \leq c \leq 10^{-4}$. In Fig. 12 it is shown that both $/_{\text{EGDM}}$ and $/_{\text{MMA}}$ increase with $\hat{\sigma}$ and c ,