Field-induced detrapping in doped organic semiconductors with Gaussian disorder and different carrier localizations on host and guest sites

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For organic host-guest systems with a low fraction of guest sites, i.e., the trap-limited case, field-induced detrapping of charge carriers is studied via master equation calculations under the assumption of Miller-Abrahams rates and two Gaussian distributions of uncorrelated energy levels. Among existing descriptions of carrier redistributions in the presence of an electric field, the effective temperature derived by F. Jansson, S. D. Baranovskii, F. Gebhard, and R. Österbacka [Phys. Rev. B **77**, 195211 (2008)] for pure host materials shows the best agreement with the simulation results. The detrapping description based on carrier heating is extended to the case that the two material-specific hopping rate parameters ν_0 (attempt frequency) and α (decay constant or inverse localization length of charge carriers) are different for host and guest sites.

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I. INTRODUCTION

During the past years, the interest in organic semiconductors has rapidly increased. Besides their use in lasers [1,2], solar cells [3,4], and holograms [5], the probably most promising application is the organic light-emitting diode (OLED). Although the conductivity of OLEDs is significantly lower than that of inorganic semiconductors [3], they are sought after for their high emission efficiency, fast response, low driving voltage, and simple fabrication [6]. Due to the use of dye dopants to tune color and efficiency [7] as well as the presence of parasitic traps [8], proper theoretical models for the charge carrier transport in OLEDs in the presence of guest sites are desired.

OLEDs consist of amorphous organic materials, in which carriers are localized on single sites, which can be small molecules or functional groups of polymers. Carrier transition between such sites with energy difference $E_j - E_i$ and distance R_{ij} is in theoretical studies mostly described by Miller-Abrahams rates [9]

$$\nu_{ij} = \nu_0 \exp\left(-2\alpha R_{ij} - \frac{E_j - E_i + |E_j - E_i|}{2 k_B T}\right). \quad (1)$$

In this equation, α denotes the inverse localization length of a charge carrier on a site and the prefactor ν_0 can figuratively be called attempt frequency. An early study of carrier transport based on these rates in amorphous inorganic materials was presented by Mott [10]. This analytical model, which is focused on the temperature dependence, was verified through percolation theory by Ambegaokar *et al.* [11]. The concepts used by these authors were many years later applied to amorphous organic semiconductors, first under the assumption of exponential densities of states (DOSs) [12,13], then for Gaussian densities of states [14,15], which are mostly assumed to apply to organic materials. Several other semianalytical models applicable to hopping transport in a Gaussian DOS have been suggested [16–21]. Charge transport in amorphous organic semiconductors has also been investigated in many computer simulations. At first, they were based on the Monte Carlo (MC) method [22], then the computationally more efficient master equation (ME) approach became the preferred method [23]. The carrier mobility in amorphous organic semiconductors strongly depends on temperature T, electric field F, and carrier concentration n [24–26]. A dependence on T and n for low fields can be directly derived from all aforementioned semianalytical models and has been shown to quantitatively agree with computer simulations for several of these models [15]. A field dependence, on the other hand, has been only included in two of the semianalytical models [20,27]. Especially these two models haven been shown, however, to severely disagree with ME simulations even in the low-field regime [15,28]. Hence, the time-consuming ME or MC simulations are indispensable to determine reliable field-dependent mobility values. Widely used parametrizations of the field dependence resulting from Miller-Abrahams rates in a Gaussian DOS have been derived via MC simulations at low carrier concentrations in the case of uncorrelated [22] and correlated [29] energetic disorder and via ME simulations also at high carrier concentrations for both disorder types [30,31].

While disordered, pure host systems have been widely studied, little attention has been drawn to host-guest systems so far. An early examination of organic materials intentionally doped with traps was performed by Hoesterey and Letson [32], who used a simple model depending on temperature, trap depth, and concentration to explain measurements of transient photocurrents. One of the first Monte Carlo simulations within this topic considered the transient carrier propagation in a doped device after application of a voltage [33]. While the subject was dropped for the subsequent years, several researchers recently started to apply the models and simulation methods mentioned before to host-guest systems: Three semianalytical models were applied to these systems [34,35] and two computer studies based on ME simulations were performed [36,37]. The results were in agreement with experimental findings that the mobility decreases for increasing guest concentration, as long as carrier transport is determined by hopping between host sites [38]. In this regime, transport is called trap-limited, since guest sites merely act as traps. As soon as direct guest-to-guest hopping starts to occur, the mobility reaches its minimum and increases with further increasing guest site concentration. Both ME-based studies also considered the field dependence. They explicitly verified

that the well-known expression

$$\mu = \mu_h \frac{n_h}{n_h + n_g} \tag{2}$$

for the mobility μ in the case of trap-controlled transport, with n_h (n_g) denoting the concentration of carriers residing on host (guest) sites and μ_h the mobility of the pristine host material, is valid for arbitrary values of n, T, and F in the case of hopping in a Gaussian host-guest system. Taking all dependencies into account, Eq. (2) for these systems reads

$$\mu(n,F,T) = \mu_h(n_h(n,F,T),F,T)\,\frac{n_h(n,F,T)}{n_h(n,F,T)+n_g(n,F,T)}, \tag{3}$$

with the total carrier concentration $n = n_h + n_g$. For realistic trap depths, the second factor can show an even stronger dependence on temperature and carrier concentration than the mobility of the pristine host material. The second factor also introduces an additional field dependence of considerable magnitude. Cottaar *et al.* suggested a parametrization for this latter dependence based on field-induced spreading of chemical potentials [37]. To our knowledge, this parametrization was the only attempt so far to quantify the field dependence of carrier mobility in disordered organic semiconductors in the trap-controlled regime.

In this paper, we will focus on the field dependence of the ratio $n_h/(n_h + n_g)$ as it has been studied the least so far and can dominate the behavior of real devices. Unlike previous investigations, we consider different attempt frequencies $\nu_{0,h/g}$ and inverse carrier localizations $\alpha_{h/g}$ for host and guest sites. Section II starts with the explanation of the bulk properties, the numerical method, and the effective temperature models. Section III A explains the optimal set of numerical parameters for the ME simulations. In Sec. III B, we show that the variation of attempt frequencies and carrier localizations for guest sites can be effectively reduced to the variation of one of these two parameters. In Sec. III C, the simulation results for equal and different values of α_h and α_g are presented and compared to several parametrization schemes.

II. THEORY

We consider a cubic lattice of length L in each direction, the sites of which are assumed to have the DOS

$$g(E) = (1-x)\,g_h(E) + x\,g_g(E), \tag{4}$$

with x denoting the guest site fraction and

$$g_h(E) = \frac{N}{\sigma_h\sqrt{2\pi}}\exp\left(-\frac{E^2}{2\sigma_h^2}\right), \tag{5}$$

$$g_g(E) = \frac{N}{\sigma_g\sqrt{2\pi}}\exp\left(-\frac{(E+\Delta)^2}{2\sigma_g^2}\right) \tag{6}$$

the Gaussian DOS of host and guest sites, respectively. The random energy levels are uncorrelated. $N = 1/a^3$ is the spatial site density, σ_i are the respective widths, and Δ is the trap depth. All lengths throughout this work are given in units of the lattice constant a, all inverse localization lengths α in units of a^{-1}. Once the lattice is assigned, the hopping from a certain site i to j is described by a generalized Miller-Abrahams (GMA) rate

$$\nu_{ij} = \sqrt{\nu_{0,i}\,\nu_{0,j}} \times \exp\left[-(\alpha_i+\alpha_j)\,R_{ij} - \frac{E_j - E_i + |E_j - E_i|}{2\,k_B T}\right]. \tag{7}$$

An important numerical parameter is the cutoff radius r_m of the sphere containing all potential hopping neighbors. Hopping rates at the border of the cube are treated by imposing periodic boundary conditions. The energy E_i of each site is the superposition of the electrostatic potential due to the electric field F and an the equilibrium energy which is randomly chosen according to the distribution $g(E)$.

With the hopping rates and a given number of charge carriers, the carrier occupancies p_i can be determined by the master equation

$$\sum_{j\neq i}[\nu_{ij}\,p_i(1-p_j) - \nu_{ji}\,p_j(1-p_i)] = 0. \tag{8}$$

This equation was first applied to organic materials by Yu *et al.* [23]. Instead of the method employed in their work, we use, however, Newton's method for its solution as it was already done by Szymanski *et al.* [39]. Coulomb interaction between the carriers is neglected. For the considered relative carrier concentration n/N in the range between 10^{-5} and 10^{-4}, this simplification has no influence on the mobility [40]. The ratio $n_h/(n_h+n_g)$ is then easily obtained as the sum of all host site occupancies divided by the sum of all lattice site occupancies. Detrapping is the change of this ratio with increasing field.

In an attempt to parametrize the simulation results for potential use in a drift-diffusion model, we used several approaches from the literature. Our main focus was on carrier heating in Gaussian DOSs as described by Jansson *et al.* [41] according to the equation

$$T_{\mathrm{eff},h/g} = \left[T^\beta + \left(\gamma\frac{e\,F}{\alpha_{h/g}\,k_B}\right)^\beta\right]^{\frac{1}{\beta}} \tag{9}$$

with $\beta = 1.54$ and $\gamma = 0.64$. This expression was verified for pure host systems by simulations and measurements [42] and it can be easily applied to host-guest systems with $\alpha_h = \alpha_g$ and $\nu_{0h} = \nu_{0g}$. Considering particle number conservation

$$n = n_h + n_g = (1-x)\int_{-\infty}^{\infty} dE\,g_h(E)\,f(E,E_F,T_{\mathrm{eff},h}) + x\int_{-\infty}^{\infty} dE\,g_g(E)\,f(E,E_F,T_{\mathrm{eff},g}) \tag{10}$$

with the Fermi distribution f, the Fermi energy E_F is uniquely determined since the total charge carrier density n is given. One can then reinsert E_F into the host carrier density n_h and calculate the detrapping by n_h/n.

It was claimed by Cottaar *et al.* [37] that the assumption of carrier heating strongly overestimates field-induced detrapping, and they suggested a field-dependent spreading of chemical potentials instead. However, they only compared their results to an expression for field-induced carrier heating

which had been derived by Preezant and Tessler based on the so-called energy space master equation (ESME) [43]. This simulation approach calculates an energetic distribution of carriers in the volume and assigns it to each lattice site. Hence, it differs conceptually from the ME approach, which assigns randomly chosen but discrete energy levels to the lattice sites and calculates carrier occupancies for these sites. It is shown in the following section that, for a host-guest system with $\alpha_h = \alpha_g$ and $\nu_{0,h} = \nu_{0,g}$, detrapping parametrization based on the effective temperature from ME simulations, though far from perfect, is clearly superior to fits based on the ESME-based effective temperature or the spreading of chemical potentials.

This leads to the question of how detrapping in host-guest systems with $\alpha_h \neq \alpha_g$ or $\nu_{0,h} \neq \nu_{0,g}$ can be described. It is also shown in the next section that this problem can be reduced to $\alpha_h \neq \alpha_g$. Hence, Eq. (9), which only contains a localization length and no attempt frequency, can still be used as a starting point. A first possibility to account for $\alpha_h \neq \alpha_g$ would be the use of Eq. (10) with $T_{\mathrm{eff},h} \neq T_{\mathrm{eff},g}$. This approach, from here on referred to as model 1, implies separate carrier heating in host and guest DOSs unaffected by each other but thermal quasiequilibrium of all charge carriers in the volume. This assumption, however, leads to the prediction that a decrease of α_g (a measure for carrier localization on guest sites) would result in a reduction of field-induced detrapping for a given α_h. Since this prediction contradicts any intuition, we suggest a second model, which is chosen to fulfill three important conditions: First, it takes into account contributions from host-host, guest-guest, and host-guest interactions to the energetic redistribution of carriers. Second, reduction of α_g and reduction of α_h lead both to enhanced field-induced detrapping if the trap depth Δ is large. Third, the expression is equivalent to Eqs. (9) and (10) for $\alpha_h = \alpha_g$.

The suggested expression is based on the well-known ratio n_g/n_h in the Boltzmann limit without an electric field [35]:

$$\frac{n_g}{n_h} = \frac{N_g}{N_h} \exp\left[-0.5\left(\frac{\sigma_h}{k_B T}\right)^2 + 0.5\left(\frac{\sigma_g}{k_B T}\right)^2 - \frac{\Delta}{k_B T}\right]. \tag{11}$$

Three different effective temperatures are now inserted in this expression:

$$\frac{n_g}{n_h} = \frac{N_g}{N_h} \exp\left[-0.5\left(\frac{\sigma_h}{k_B T_{\mathrm{eff},h}}\right)^2 + 0.5\left(\frac{\sigma_g}{k_B T_{\mathrm{eff},g}}\right)^2 - \frac{\Delta}{k_B T_{\mathrm{eff},\Delta}}\right]. \tag{12}$$

$T_{\mathrm{eff},h}$ and $T_{\mathrm{eff},g}$ are calculated from α_h and α_g, whereas for $T_{\mathrm{eff},\Delta}$ we use an averaged decay constant $\alpha_\Delta = 0.5(\alpha_h + \alpha_g)$. This parametrization is supposed to include the interaction between host and guest sites. With such an expression in combination with a correction factor to approximate deviations from the Boltzmann limit at higher carrier concentrations, we have already successfully modeled temperature-dependent IV curves of lowly doped organic diodes [44].

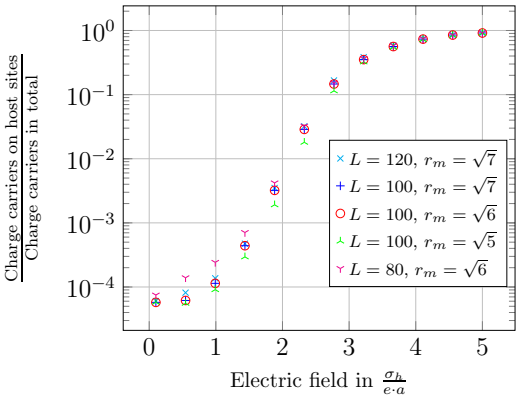

FIG. 1. (Color online) Convergence analysis for $(\alpha_h, \alpha_g) = (3,3)$. Based on these results, the numerical parameter set $(L, r_m) = (100, \sqrt{6})$ was chosen for subsequent calculations.

III. DATA ANALYSIS

A. Convergence

Prior to a discussion of physical behavior, a proper convergence analysis for L and r_m had to be performed. We considered the most critical parameter combination within our study ($\nu_{0,g/h} = 1$, $\alpha_{g/h} = 3$), determined the sufficient set of numerical arguments, and used them for all other simulations as well.

Based on the findings in Fig. 1, we chose $L = 100$ and $r_m = \sqrt{6}$. Three regimes can be distinguished in the plot: While the wrong choice of lattice size leads to the highest error at low electric fields, the maximum hopping distance r_m has the highest influence at intermediate fields around $2\frac{\sigma_h}{e \cdot a}$. For high fields, at which the percolation character of carrier transport vanishes, the choice of numerical parameters becomes less critical.

B. Compensation of $\nu_{0,g}$ and α_g

To reduce the effort of analyzing host-guest systems with different $\nu_{0,g}$ and α_g and to describe detrapping based on

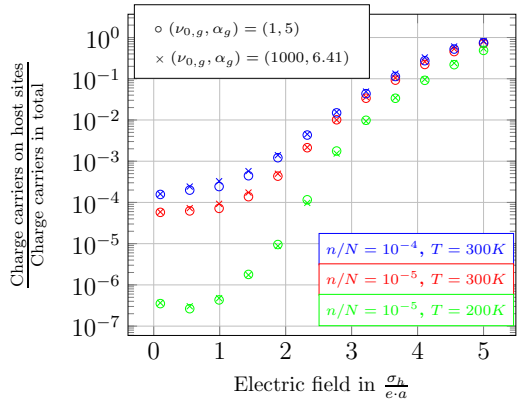

FIG. 2. (Color online) Compensation of variations of $\nu_{0,g}$ and α_g according to Eq. (14) for three different combinations of temperature and carrier concentration at $r_m = \sqrt{6}$ and host site parameters $(\nu_{0,h}, \alpha_h) = (1,5)$.

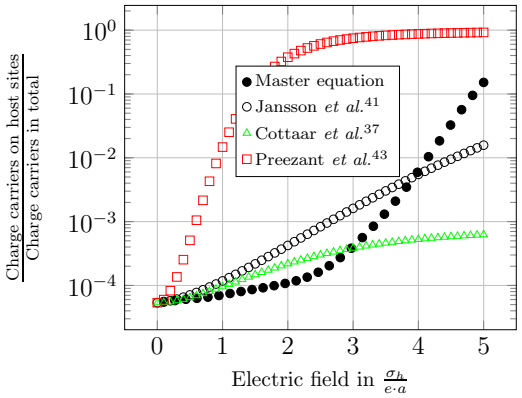

FIG. 3. (Color online) Results of our master equation for the parameter set from Table I and $\alpha_h = \alpha_g = 10$ compared to three existing models for energetic redistribution of carriers: the effective temperature based on the ESME approach proposed by Preezant and Tessler [43], the effective temperature based on ME results as parametrized for pure host systems by Jansson *et al.* [41], and the spreading of chemical potentials as claimed by Cottaar *et al.* [37] based on their ME simulations of host-guest systems.

Eq. (9), which does not include ν_0, we examined the compensation of both parameters by varying them simultaneously and checked whether the investigation could be effectively reduced to α_g. Detrapping is governed by hops which include one guest and one host site. Recasting the according GMA rate [Eq. (7)] leads to

$$\nu_{ij} = \sqrt{\nu_{0,h}}\,\exp\left(-\alpha_h\,R_{ij} - \frac{E_j - E_i + |E_j - E_i|}{2\,k_B T}\right) \times \sqrt{\nu_{0,g}}\,\exp\left(-\alpha_g\,R_{ij}\right). \tag{13}$$

For a given set of host material parameters, two pairs of guest material parameters, $(\nu_{0,g,a},\alpha_{g,a})$ and $(\nu_{0,g,b},\alpha_{g,b})$, were chosen according to the equation

$$\sqrt{\nu_{0,g,a}}\exp\left(-\alpha_{g,a}\,r_m\right) = \sqrt{\nu_{0,g,b}}\exp\left(-\alpha_{g,b}\,r_m\right), \tag{14}$$

with r_m denoting the previously determined maximum hopping distance.

Figure 2 shows that a variation of $\nu_{0,g}$ can be replaced by a variation of α_g via Eq. (14) for the considered parameter range, hence the condition $\nu_{0,h} = \nu_{0,g} = 1$ was kept fixed in all subsequent simulations and only α_h and α_g were varied.

C. Comparison of master equation results with theoretical models

Before the analysis of $\alpha_h \neq \alpha_g$, we compared ME simulation results for the extensively investigated [36,37] case of $\alpha_h = \alpha_g = 10$ with three existing models of carrier redistribution under an electric field. The comparison is shown in Fig. 3 (see also Table I). The model published by Cottaar *et al.* [37], which assumes a Gaussian distribution of the chemical potential, is close to the ME results for low and intermediate fields but deviates significantly for high fields. This deviations can be explained by the fact that this model assumes an upper limit for the spreading of chemical potentials and thus for the broadening of the Fermi distribution. ME simulations however reveal an arbitrarily strong broadening of the distribution function resulting in a nearly uniform distribution for very high fields as shown in Fig. 7. The model by Preezant and Tessler [43] severely overestimates field-induced detrapping as already stated [37]. This is no surprise since ESME simulations predict a much higher effective temperature than ME simulations. The effective temperature as parametrized by Jansson *et al.* [41] based on ME simulations, on the other hand, captures the overall tendency for the whole field range better than the other models. Additionally, our ME simulations for $\alpha_h = \alpha_g = 5$, which are presented in Fig. 4, show that the field dependence of detrapping indeed scales

TABLE I. Parameters used for all simulations if not explicitly stated otherwise.

a	$\sigma_{h,g}$	T	x	Δ	n/N	$\nu_{0,h/g}$
10^{-9} m	0.1 eV	300 K	0.01	$-4\sigma_h$	10^{-5}	1

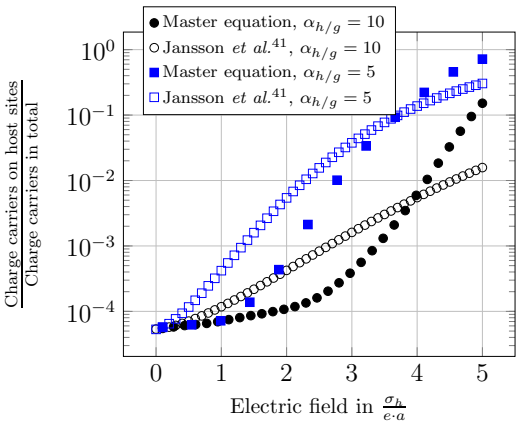

FIG. 4. (Color online) Comparison of our ME results to calculations of detrapping based on the effective temperature derived by Jansson *et al.* [41] for two different sets of $\alpha_h = \alpha_g$. It is revealed that the field dependence of detrapping scales in the same way with α as the effective temperature in pure host systems.

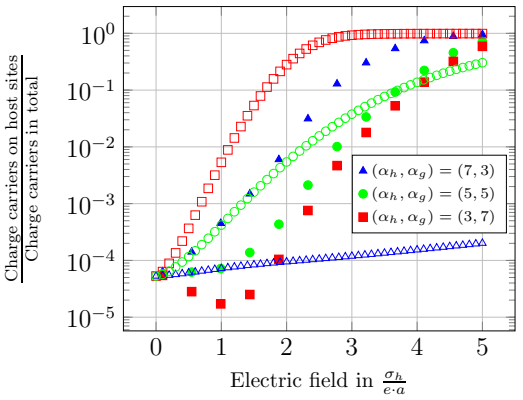

FIG. 5. (Color online) Comparison of ME results (full symbols) to model 1 (open symbols). For $\alpha_h \neq \alpha_g$, the model strongly deviates from the simulation results and even predicts opposite tendencies.

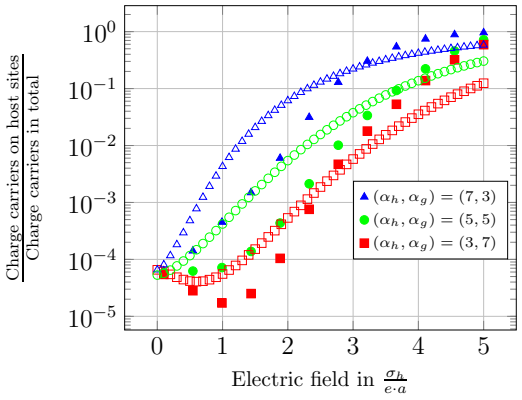

FIG. 6. (Color online) Comparison of ME results (full symbols) to model 2 (open symbols). Introducing a "mixed" carrier heating approach leads to a drastic improvement compared to model 1.

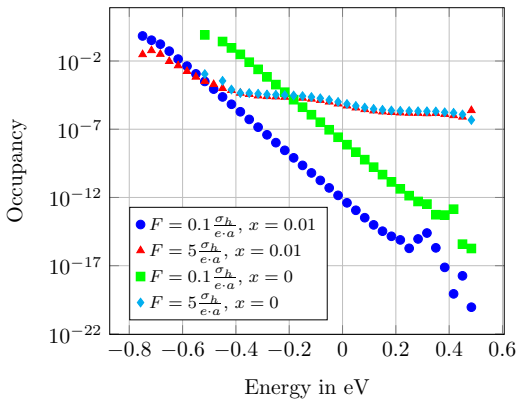

FIG. 7. (Color online) Energetic distribution of charge carriers for a pure host and a host-guest system with $\alpha_{h/g} = 10$. At high fields, both distributions become nearly identical and uniform among all energies.

with α as expected from Eq. (9). Thus, the usual scaling of the electric field as eFa/σ is inadequate and the influence of carrier localization on the characteristics of charge transport in OLEDs has been underestimated so far.

After the verification that detrapping can be at least roughly characterized by carrier heating, we extended this model to the case of different carrier localizations for host and guest sites. Figures 5 and 6 show three exemplary cases for (α_h,α_g): (3,7), (7,3), and (5,5), the last of which is already included in Fig. 4. The ME results reveal how the detrapping and hence the mobility are changing if one varies α_h and α_g while leaving the sum $\alpha_h + \alpha_g$ constant. Figure 5 compares the ME results with the previously explained model 1 and shows that the assumption of two separate Fermi distributions with one common chemical potential for different α_h and α_g is completely unjustified. As already expected, even the predicted tendency of this model is the opposite of the simulation results. Model 2, the results of which are depicted within Fig. 6, shows a much better accordance, even though the deviation between this model and the ME simulation results peaks at one order of magnitude. Characteristic features of the ME results are, however, explained by this model, including even the local minimum of the fraction of free carriers for (α_h,α_g) = (3,7) at $F = 1 \frac{\sigma_h}{e \cdot a}$, which can be qualitatively explained through the exponent in Eq. (12).

D. Energetic distribution of charge carriers

To illustrate field-induced carrier heating, Fig. 7 compares the energetic distribution of a pure host system ($x = 0$) with a system containing guest sites ($x = 0.01$) for low and high fields at (α_h,α_g) = (10,10). For a vanishing field of $0.1 \frac{\sigma_h}{e \cdot a}$, a constant shift between the two respective distributions can be seen, which indicates that guest sites, if present, are mostly occupied. For high fields, the distribution functions change to approximately uniform distributions as expected for very high effective temperatures. Accordingly, the curves for $x = 0$ and $x = 0.01$ are practically identical, which means that the presence of a low fraction of guest sites becomes irrelevant at high fields.

IV. CONCLUSION

For the examination of detrapping in a disordered host-guest system with hopping rates of the Miller-Abrahams type, the consideration of different attempt frequencies and carrier localizations could, within the investigated parameter range, be effectively reduced to the consideration of different carrier localizations. A subsequent comparison of the master equation results with parametrization schemes from the literature revealed that only the effective temperature proposed by Jansson *et al.* [41] captures the tendency for field-induced detrapping if equal decay constants for host and guest sites are assumed. For unequal decay constants, we have presented two different attempts to model the field-dependent behavior. The first one, assuming two different effective temperatures, failed. The second model, including a third effective temperature, which depicts the interaction between host and guest sites, gave a good approximation of the exact results from the master equation. Our findings underline the importance of decay constants for the field dependence of mobility in host-guest systems, which has been underestimated so far. A detrapping parametrization which does not only predict the tendency but also the quantitative progression is still an open problem. The lack of such a parametrization for arbitrary material properties renders drift-diffusion simulations virtually useless and makes device models based on master equation or Monte Carlo simulations a necessity for all OLEDs involving trap-limited carrier transport.

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