Field-induced detrapping in disordered organic semiconducting host-guest systems

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In a disordered organic semiconducting host-guest material, containing a relatively small concentration of guest molecules acting as traps, the charge transport may be viewed as resulting from carriers that are de-trapped from the guest to the host. Commonly used theories include only detrapping due to thermal excitation, described by the Fermi-Dirac (FD) distribution function. In this paper, we develop a theory describing the effect of field-induced detrapping (FID), which provides an additional contribution at finite electric fields. It is found from three-dimensional simulations that the FID effect can be described by a field-dependent generalized FD distribution that depends only on the shape of the host density of states (DOS) and not on the guest DOS. For the specific case of a Gaussian host DOS, we give an accurate and easy-to-use analytical expression for this distribution. The application of our theory is demonstrated for sandwich-type devices under conditions typical of organic light-emitting diodes.

I. INTRODUCTION

In the rapidly emerging field of organic electronics use is made of disordered organic semiconductors such as π-conjugated polymers or small molecules, in which transport takes place by hopping of charge carriers between states localized at specific sites. Host-guest systems play an important role within the field of organic electronics and are encountered in several applications. In organic light-emitting diodes (OLEDs), the emissive layers are often doped, and both phosphorescent[1] and fluorescent[2] guest emitters can behave as traps of charge carriers. Also, doped organic layers can assist in charge injection.[3] Other applications of host-guest systems are in organic field-effect transistors,[4] xerography,[5] and organic lasers.[6] But also nominally undoped systems can sometimes act as host-guest systems. In particular, many organic semiconductors contain electron traps, often caused by contact with oxygen,[7] leading to vastly reduced electron mobilities as compared to hole mobilities.[8–11]

Charge transport in host-guest systems has been extensively studied since the nineteen sixties.[12] The first semianalytical result was given by Hoesterey and Letson (HL),[13] based on a system with states at only two energy levels: a transport state (host) and a trap state (guest). Within their approach, the population of host and guest states is obtained assuming local thermal equilibrium, i.e., using the Fermi-Dirac (FD) distribution function, and the charge transport is determined by the fraction of carriers, the "free" carriers, that occupy the host density of states (DOS). The HL model shows that at extremely low guest concentrations the transport is dominated by hopping in between host sites, so that the presence of the guest can be ignored and that as the guest concentration increases hopping between host and guest sites becomes important, leading to trapping of charge carriers by the guest and a dramatic reduction in the charge-carrier mobility.[14] The model loses its validity when at high guest concentrations direct hopping in between guest sites starts to occur, leading to an increase in the mobility until eventually the charge transport is fully dominated by guest-to-guest hopping. This concept of thermal detrapping may be readily generalized to more complex shapes of the host and guest DOS.[15,16] The dependence of the effective mobility on the charge-carrier density is then not only related to the fraction of detrapped charge carriers but also to the density dependence of the mobility in the host DOS.[17–19] However, the model is only valid in the limit of zero electric field. At finite values of the electric field, the fraction of free charge carriers exceeds the fraction that is obtained from the FD distribution function. This "field-induced detrapping" (FID) effect gives rise to an additional contribution to the mobility. So far, this effect has only been studied for specific host-guest systems using various semianalytical approximations[20–26] and a general model for the effect that may be readily used in drift-diffusion device simulations of organic electronic devices is lacking.

In this paper, we will develop an accurate and easy-to-use model for the mobility in host-guest systems with a Gaussian host DOS and a general guest DOS, including the effect of FID. The model is valid in the regime of low guest concentrations, where guest-to-guest hopping can be neglected. The approach is based on the results of transport modeling using a master-equation (ME) approach. In an earlier study,[27] it was already found that the effect of FID on the mobility as obtained from ME modeling is significantly different from the effect as predicted by a semianalytical effective-medium theory. Using the ME modeling results, we show that the HL model can be extended to finite values of the electric field by using a generalized FD distribution function that depends only on the shape of the *host* DOS and the electric field, and not on the guest DOS. Although one might loosely say that the field gives rise to a "hot" out-of-equilibrium distribution, we show that the shape of the generalized FD function is not well represented by introducing an effective field-enhanced temperature. In order to facilitate applications of our work in device simulations, we present analytical expressions for the generalized FD function for a wide range of widths of the Gaussian DOS. We furthermore demonstrate the role of FID

in sandwich-type metal/organic semiconductor/metal devices.

In Sec. II, we develop our generalized HL model for the mobility in host-guest systems. In Sec. III, parametrized expressions are given for the generalized FD distribution function, with a form based on the observed spatial structure of the field-dependent occupation probabilities. An application to devices is given in Sec. IV. Finally, a summary, conclusions, and an outlook are given in Sec. V.

II. GENERALIZED HOESTEREY-LETSON DETRAPPING MODEL

We consider host-guest systems with a normalized total DOS of the form

$$g(\varepsilon) = (1-x)g_{\mathrm{h}}(\varepsilon) + xg_{\mathrm{g}}(\varepsilon), \tag{1}$$

where g_{h} is the normalized Gaussian DOS of the host, with width σ, g_{g} is the normalized guest DOS and x is the guest-molecule concentration. The total hopping site density is $N_{\mathrm{t}} \equiv a^{-3}$, with a the average intersite distance. The total, host and guest carrier densities are n, n_{h}, and n_{g}, respectively, and the corresponding carrier concentrations c, c_{h}, and c_{g} are defined by normalization with respect to the site density N_{t}. Within the standard HL model, applicable in the zero-field limit, the mobility at a certain carrier concentration is given by $\mu(c) = (c_{\mathrm{h}}/c)\mu_{\mathrm{h}}(c_{\mathrm{h}})$, where $\mu_{\mathrm{h}}(c_{\mathrm{h}})$ is the mobility in the pure host material at a carrier concentration c_{h}. This concentration may be found by solving the following set of equations:

$$c = xc_{\mathrm{g}} + (1-x)c_{\mathrm{h}} \tag{2}$$

and

$$c_{\mathrm{g}} = \int_{-\infty}^{\infty} g_{\mathrm{g}}(\varepsilon)p[\varepsilon, \varepsilon_{\mathrm{F}}(c_{\mathrm{h}}, T)]d\varepsilon \tag{3}$$

with $p[\varepsilon, \varepsilon_{\mathrm{F}}(c_{\mathrm{h}}, T)]$ the FD distribution function

$$p[\varepsilon, \varepsilon_{\mathrm{F}}(c_{\mathrm{h}}, T)] = \frac{1}{\exp\{[\varepsilon - \varepsilon_{\mathrm{F}}(c_{\mathrm{h}}, T)]/kT\} + 1}, \tag{4}$$

which gives the probability of a charge carrier being present at a site with energy ε at a specific host carrier concentration- and temperature-(T-) dependent Fermi energy $\varepsilon_{\mathrm{F}}(c_{\mathrm{h}}, T)$.

In order to investigate the effect of an electric field on the mobility, we have carried out calculations of the mobility using a master-equation approach analogous to that described earlier for the case a monomodal Gaussian DOS.[18] The transport process is described as a result of hopping between sites on a cubic lattice of $L \times L \times L$ sites with periodic boundary conditions and with lattice spacing a. The guest sites are randomly distributed, with site energies that are randomly taken from the guest DOS, and the energies on the remaining (host) sites are taken randomly from the host DOS. There are thus no spatial correlations between the energies on neighboring sites. Within this approach, the hopping probability between an occupied site i and an unoccupied site j is assumed to be given by the Miller-Abrahams expression[28]

$$\omega_{ij} = \begin{cases} \nu_0 \exp(-2\alpha R_{ij} - \Delta\varepsilon_{ij}/kT), & \text{for } \Delta\varepsilon_{ij} \geq 0, \\ \nu_0 \exp(-2\alpha R_{ij}), & \text{for } \Delta\varepsilon_{ij} < 0, \end{cases} \tag{5}$$

where ν_0 is the hopping attempt frequency, α the inverse of the wave-function overlap distance, R_{ij} the distance between the sites, and $\Delta\varepsilon_{ij}$ is the energy difference, taking the field F into account:

$$\Delta\varepsilon_{ij} = \varepsilon_j - \varepsilon_i - eFR_{ij,x} \tag{6}$$

with e the elementary charge and $R_{ij,x}$ the distance between the two sites as measured along the field (x) direction. In the actual calculations the hop rate is given by $\omega_{ij}p_i(1-p_j)$, taking into account the probability p_i that site i is occupied and the probability $1-p_j$ that site j is empty. We first find the occupational probabilities p_i by solving the so-called ME, which states that the flow of charges into and out of every site must be equal

$$\sum_j \omega_{ij}p_i(1-p_j) = \sum_j \omega_{ji}p_j(1-p_i), \tag{7}$$

for all i. The current density is given by

$$J = \frac{e}{(aL)^3}\sum_{i,j} \omega_{ij}p_i(1-p_j)R_{ij,x}. \tag{8}$$

In the ME approach it is not possible to consistently take Coulomb interactions between carriers into account since the ME is an equation for the time averaged and not the actual occupational probabilities. However, at the carrier concentrations considered in this paper the effects of Coulomb interactions are not relevant.[29] As in Ref. 18, we use a value $\alpha = 10a^{-1}$ throughout the present work. For pure host transport, the resulting model, with a dependence of the mobility on temperature, electric field and carrier density as parameterized in Ref. 18, is known as the extended Gaussian disorder model (EGDM).

In host-guest systems, the attempt frequency for host-guest hopping will in general be different from that for host-host hopping. However, as long as the guest sites only act as traps this does not affect the mobility, as may be seen as follows. Within the ME approach, the relationship between the occupational probability p_i on a site i and the occupational probabilities p_j on all other sites is given by[30]

$$p_i = \frac{\sum_j \omega_{ji}p_j}{\sum_j [\omega_{ij}(1-p_j) + \omega_{ji}p_j]}. \tag{9}$$

Due to detailed-balance considerations, the attempt frequencies for host-guest and guest-host hops are equal. If site i is a guest site surrounded by host sites, a change in the host-guest attempt frequency therefore changes ω_{ij} and ω_{ji} by the same factor for all j. As a result, the numerator and denominator in Eq. (9) are changed by the same factor and p_i is unaffected. This implies that the density of trapped and free carriers does not change, so that the mobility in the host-guest system is unaffected. For simplicity, we will therefore assume that all attempt frequencies are equal.
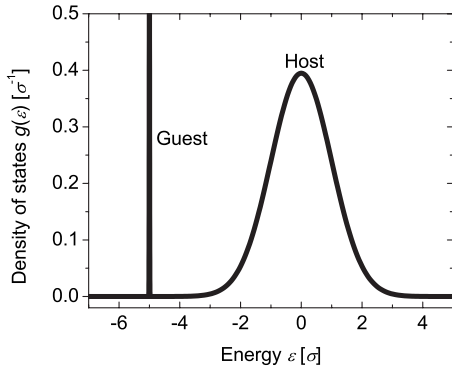
FIG. 1. Density of states for the example host-guest system introduced in Sec. II. The host sites have a Gaussian energy distribution centered around zero energy with width σ. The guest sites all have energy -5σ.

Before developing the general method, we first illustrate the effect of field-induced detrapping on the mobility by discussing as a specific example a system with a Gaussian host DOS with width σ and a δ-function shaped guest DOS at an energy distance of 5σ below the top of the host DOS. The total DOS is shown in Fig. 1. Figure 2 shows the mobility as a function of the guest concentration as calculated in the limit of zero field for a dimensionless disorder parameter $\sigma/kT=3$ and for two different values of the total carrier concentration, as calculated using the ME approach (symbols) and as obtained using the HL model (lines). The results clearly show the cross-over from a low-concentration regime in which the HL model is well applicable to the high-concentration regime in which this model fails due to the neglect of direct guest-guest hopping. The cross-over concentration is approximately 5% in the example considered. In general, this concentration would depend on the value of the wave-function decay length and on the specific values of the attempt frequencies for guest-guest, guest-host, and host-host hopping.
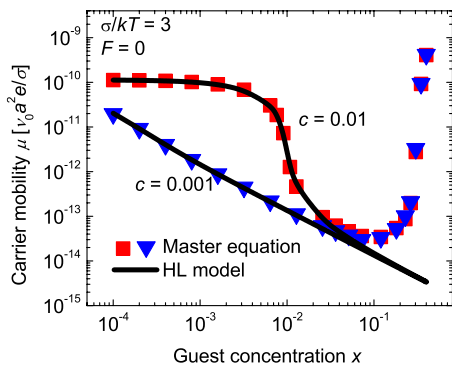

FIG. 2. (Color online) Dependence of the charge-carrier mobility μ on the guest concentration x for the example host-guest system, with $\sigma/kT=3$ and a vanishing electric field $F=0$. The upper line and squares correspond to a total carrier concentration of $c=0.01$ and the lower line and triangles to $c=0.001$. The symbols represent the results of master-equation (ME) calculations on the host-guest system while the lines represent the results of the Hoesterey-Letson (HL) model, obtained by solving Eqs. (2) and (3) with the Fermi-Dirac (FD) distribution function Eq. (4).
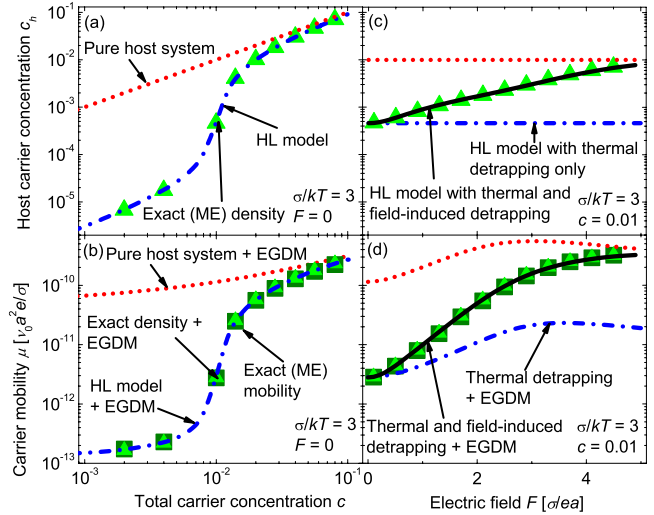

FIG. 3. (Color online) Dependence of the carrier concentration in the host c_h [(a) and (c)] and mobility μ [(b) and (d)] on the total carrier concentration c at $F=0$ [(a) and (b)] and on the electric field F at $c=0.01$ [(c) and (d)], for the example host-guest system with a guest concentration of 1% and $\sigma/kT=3$. In (a) the carrier concentration in the host is shown without taking the guest into account (dotted red line) and by applying the HL model (dashed-dotted blue line), obtained by solving Eqs. (2) and (3) with the FD distribution function Eq. (4). The light-green triangles represent the actual carrier concentration in the host as found from ME calculations for the host-guest system. In (c) the field dependence of the carrier concentration in the host is shown. Two HL model results are shown here, for thermal detrapping only [dashed-dotted blue line, based on the FD function Eq. (4)] and for thermal and field-induced detrapping [solid black line, based on Eq. (11)]. In (b) and (d) the mobilities resulting from these free carrier concentrations in the host by applying the extended Gaussian disorder model (EGDM) are shown. Also included here are the exact mobilities found from the ME calculations for the host-guest system (dark-green squares).

Figure 3 shows the host carrier concentrations and the effective mobilities for the case of a fixed guest-molecule concentration $x=0.01$. Figures 3(a) and 3(b), which give the host carrier concentrations and effective mobilities, respectively, as a function of the total carrier concentration at zero field show that the standard HL model provides an excellent prediction of the carrier-concentration dependence of the mobility. We note that already in the pure host system the mobility is slightly carrier concentration dependent and that we have used the EGDM to describe that effect. In contrast, Figs. 3(c) and 3(d), which give the host carrier concentrations and effective mobilities, respectively, as a function of the electric field at a fixed carrier concentration ($c=0.01$), show that the standard HL thermal detrapping model fails to provide an accurate description of the host carrier concentration and the carrier mobility. However, it may also be seen that an excellent prediction [light-green triangles in Fig. 3(d)] of the ME mobility [dark-green squares in Fig. 3(d)] is obtained if the mobility is calculated with the EGDM using the enhanced host carrier concentration that has been calculated using the ME approach [light-green triangles in Fig. 3(c)]. This proves that the general HL picture, within which the mobility is viewed as resulting from the fraction of car-

riers residing in host states, is still valid but that the field-enhanced host carrier concentration should be used instead of the concentration obtained assuming thermal detrapping only.

For practical device-simulation applications, within which the shape of the guest DOS is often not *a priori* clear, the ME approach used will in general be computationally too expensive and involved. Repeating it for every host-guest system one may encounter is undesirable. We argue that, as an alternative, the field-dependent host carrier concentration may be obtained by using in Eq. (3) a generalized field-dependent occupation function $p(\varepsilon; F, c_h, T)$ instead of the FD distribution function. It may be understood as follows that such a function, which should apply to both host and guest sites, indeed exists. First while the energies of host and guest sites are drawn from a different DOS, a guest site at a certain energy cannot be distinguished from a host site that happens to have the same energy. This means that one single occupation function describes the average occupational probabilities of both host and guest sites. Second, this occupation function does not depend on the shape of the guest DOS and on the guest concentration. This follows from the assumption that the presence of guest sites does not influence the charge-transport properties of the host, which is valid at the low guest concentrations that we consider in the present work.

III. FIELD-DEPENDENT OCCUPATION FUNCTION

In this section, we investigate the shape of the generalized occupation function and we develop an accurate and easy-to-use analytical expression for the specific case of a Gaussian host DOS. As a first step, ME calculations were used in order to obtain this function in a numerically exact manner for selected values of the carrier concentration, the electric field and the dimensionless disorder parameter $\hat{\sigma} \equiv \sigma/kT$. The calculations were performed using a lattice of about 10^6 sites. The occupation function then follows directly from the site-averaged occupational probabilities as a function of the site energy.

The numerical accuracy of the distribution is limited by the finite size of the lattice. It was found that the accuracy can be enhanced in an efficient way by making use of Eq. (9), which gives the occupational probability of a site i as a function of those of the surrounding sites. This expression makes it possible to calculate the average occupational probability of a site at a certain energy ε_i' from the already calculated occupational probabilities of sites surrounding a site with a different energy ε_i that was already included in the lattice considered, and from the modified hopping rates when replacing ε_i by ε_i'. By applying this procedure to multiple sites, in all cases with energies ε_i as close as possible to ε_i', and by performing an average, we find the value of the occupation function at ε_i'.

As an example, Fig. 4 (red solid line) shows the energy dependence of the occupation function $p(\varepsilon; F, c_h, T)$ for a value of the dimensionless electric field parameter $\hat{F} \equiv Fea/\sigma = 2$ for a system with $\hat{\sigma} = 3$ and $c = 3 \times 10^{-5}$. The reduction in the occupation function at low energies, as compared to the FD distribution at zero field (thin solid line), is

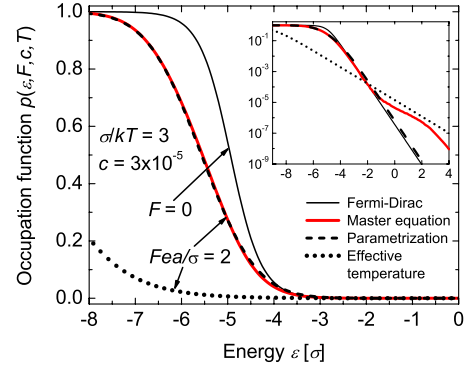
FIG. 4. (Color online) Dependence of the occupation function p on the site energy ε for electric field $F = 2\sigma/ea$, disorder strength $\sigma/kT = 3$ and carrier concentration $c = 3 \times 10^{-5}$. The red solid line shows the ME result. The dashed line shows the parametrization given by Eqs. (11)–(14) and (15a)–(15c). The dotted line shows the result of the effective temperature model of Ref. 32. The thin solid line shows the FD distribution, which is equal to the occupation function at zero field. Inset: the same, in a linear-log plot.

clearly visible. On the other hand, the occupation function is larger than the FD distribution in the energy region where the majority of the host sites are located, as may be seen in the inset of Fig. 4. This accommodates for the conservation of the total number of charges.

In order to develop an accurate parameterization of the occupation function, we have first investigated whether we could employ the concept of an effective temperature.[31–33] Indeed we observe from Fig. 4 that a finite electric field leads to a widening of the energy range in which the occupation function changes from unity to zero. The occupation function obtained using the effective-temperature model of Ref. 32, with an FD distribution using an effective temperature given by $(T_{\text{eff}}/T)^2 = 1 + [0.37Fa/(kT/e)]^2$, is indicated by the dotted line in Fig. 4. We observe that in the energy region of the host DOS this occupation function gives a reasonable description of the ME result (see inset). However, in the low energy region relevant for detrapping this description fails.

An accurate approach to parameterizing the occupation function was found after studying the spatial structure of the occupational probabilities p_i at finite electric fields. We can relate these probabilities to the site-resolved electrochemical potential $\bar{\mu}_i$ by

$$p_i = \frac{1}{\exp[(\varepsilon_i - \bar{\mu}_i)/kT] + 1}. \tag{10}$$

At $F = 0$, $\bar{\mu}_i$ is equal for all sites, and given by the Fermi energy.[34] When an electric field is applied, $\bar{\mu}_i$ is no longer equal for all sites. In order to visualize the resulting electrochemical potential distribution, we have performed ME calculations for a system with $30 \times 200 \times 200$ lattice sites, with a monomodal Gaussian DOS with a very large disorder parameter ($\sigma/kT = 20$) in order to emphasize the effects, for a large carrier concentration ($c = 0.1$), and for a relatively small dimensionless electric-field parameter ($\hat{F} = 0.01$). In the upper part of Fig. 5, the calculated electrochemical potential landscape is shown in a plane parallel to the electric field. It
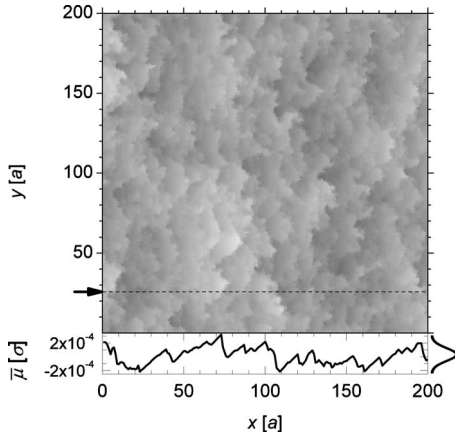
FIG. 5. Electrochemical potential landscape for $\sigma/kT = 20$ and $c = 0.1$ in a pure host system. The upper part of the figure shows the electrochemical potential $\bar{\mu}$ in a plane parallel to the electric field. A two-dimensional slice of the three-dimensional lattice is shown. An electric field $F = 0.01\sigma/ea$ is applied from left to right. Light areas correspond to a potential above and dark areas to a potential below the Fermi level. The lower part of the figure shows the electrochemical potential along the path indicated by the arrow. The resulting Gaussian distribution of $\bar{\mu}$ is sketched in the bottom right.

is clearly visible that in most regions the potential gradually rises in the direction of the field. In between these "ramps," we find abrupt "cliffs" where the potential suddenly drops. This behavior is even more clearly visible in the lower part of the figure, which shows the electrochemical potential along the one-dimensional path in the direction of the field indicated in the upper part of the figure by an arrow. The observed spatial variation in the electrochemical potential is typical for the percolative character of the charge transport in disordered systems of the type studied here.

The electrochemical potential landscape depicted by Fig. 5 suggests that the occupation function may be viewed as a result of a distribution of electrochemical potential values, related to the distribution of the sizes of the gradually rising ramps. Very large and very small values of the electrochemical potential, as compared to the average, would then correspond to those very rare large ramps that result from a major
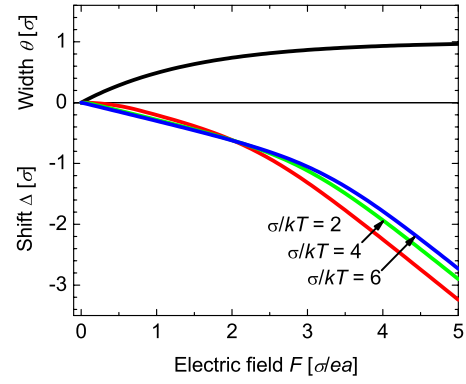

FIG. 6. (Color online) Dependence on the electric field F of the width θ and shift Δ in the parameterized occupation function Eqs. (11)–(14) and (15a)–(15c), for three dimensionless disorder strengths.

local "obstacle" in the energy landscape. We now make the approximation that the electrochemical potential of individual sites follows a statistical distribution $f(\bar{\mu}; F, c_h, T)$ that is independent of the energy of those sites,[35] so that the occupation function may be expressed as

$$p(\varepsilon; F, c_h, T) = \int_{-\infty}^{\infty} \frac{1}{\exp[(\varepsilon - \bar{\mu})/kT] + 1} f(\bar{\mu}; F, c_h, T) d\bar{\mu}. \tag{11}$$

We find that this approach indeed provides an excellent description of the occupation function if a Gaussian distribution of the electrochemical potential is taken

$$f(\bar{\mu}; F, c_h, T) = \frac{1}{\theta(F)\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left[\frac{\bar{\mu} - \varepsilon_F(c_h, T) - \Delta(F,T)}{\theta(F)}\right]^2\right) \tag{12}$$

with a field-dependent width

$$\theta(F) = [1 - \exp(-0.67|\hat{F}|)]\sigma, \tag{13}$$

and with a shift $\Delta(F, T)$ of the center away from the Fermi energy, which is parametrized by

$$\Delta(F,T) = \begin{cases} -\tau(T)\hat{F}^2 & \text{for } |\hat{F}| < 0.15/\tau(T), \\ \Delta_0(F,T) - \Delta_0(0.15/\tau(T),T) - 0.0225/\tau(T) & \text{otherwise,} \end{cases} \tag{14}$$

with

$$\Delta_0(F,T) = 0.35\chi(T) - 0.65|\hat{F}|$$
$$- \log\{2\cosh[1.05(|\hat{F}| - \chi(T))]\}/3, \tag{15a}$$

$$\tau(T) = 0.214 \times \exp[0.57(\hat{\sigma} - 2)^{1.428}], \tag{15b}$$

$$\chi(T) = 2.07 + 0.225\hat{\sigma} - |0.34 - 0.085\hat{\sigma}|. \tag{15c}$$

The dependence of θ and Δ on the dimensionless electric field $\hat{F}$ is shown in Fig. 6. In the zero-field limit the parametrized occupation function reduces to the Fermi-Dirac distribution. At small fields, θ varies linearly with the field. However, it may be verified that the effect on the occupation function and on the mobility is of second order in the field,

as should be the case. For high fields, the width of the distribution of electrochemical potentials becomes equal to the width of the DOS, as might have been anticipated from the fact that in that limit all states participate equally in the transport process. Interestingly, the parametrizations for θ and Δ are independent of the carrier concentration. This is in agreement with the observation that the field dependence in a pure host system can be taken into account in the EGDM by an enhancement factor that does not depend on the carrier concentration.[18]

Figure 4 shows that the approach indeed yields a very accurate description of the occupation function in the low-energy region for the example system studied. In general, the parameterization is accurate for the range of energies ε where $p \gtrsim 0.001$. Significant relative deviations of the occupational probabilities of guest sites only occur at high energies where $p \lesssim 0.001$.[36] For a guest concentration within the range of validity of the present model, a few percent at maximum, the maximum (worst-case) error in the space-charge concentration on the guest sites is then on the order of 10^{-5} electron charges per site. In all practical situations this is sufficiently small to give a negligible contribution to the electric field, so that it is expected that in all practical device-modeling studies our parameterization scheme can be safely applied.

The parameterization yields accurate predictions for the host carrier concentration and hence for the charge-carrier mobility in host-guest systems. For the example host-guest system discussed in the previous section, this is shown in Figs. 3(c) and 3(d) (solid lines). The parametrization of the occupation function given in the present section is valid in the case of a Gaussian host DOS and when Miller-Abrahams hopping rates are used. However, the method presented here can be easily extended to other systems, such as an exponential host DOS or hopping rates as described by the Marcus theory.[37]

IV. DEVICE APPLICATIONS

In order to demonstrate the effect of field-induced detrapping on the current density J in devices, we apply the model to sandwich-type single-layer and single-carrier devices based on an organic semiconductor with a bimodal Gaussian DOS with equal widths of the host and guest DOS. The mean energy of the guest molecules is chosen 0.65 eV below that of the host molecules, and for the guest concentration x =0.01 is taken. These values are realistic for emissive host-guest systems used in OLEDs. The other parameters determining the charge transport are taken equal to those measured for the hole transport in a polyfluorene derivative: σ =0.13 eV, a=1.19 nm, ν_0=6.28×10^{18} s^{-1}, and a relative dielectric constant ε_r=3.2.[38] Figure 7 shows that also for this more realistic host-guest system, as compared to the system discussed in the previous sections, the model yields an accurate description of the field-dependent mobility. The arrow at the field-axis indicates the electric field F=0.11 V/nm that corresponds to a dimensionless field $\hat{F}$=1. Under realistic conditions, fields up to approximately 0.15 V/nm (i.e., 15 V across a 100 nm device) can occur. Neglecting field-induced
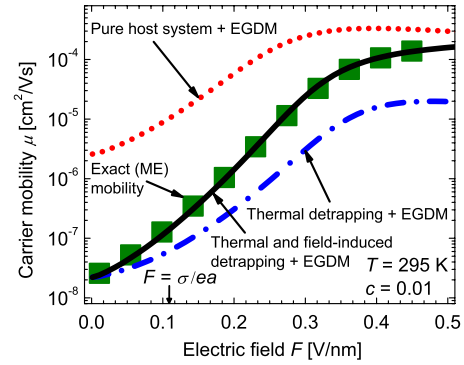

FIG. 7. (Color online) Dependence of the room-temperature mobility on the electric field for the realistic host-guest system described in Sec. IV, for a total carrier concentration c=0.01. See Fig. 3 for a description of the lines and symbols.

detrapping (dashed-dotted curve) would thus underestimate the mobility by a factor up to approximately 3. In view of the high sensitivity of the performance of OLEDs to the balance between the hole and electron mobilities, the effect may thus be regarded as quite significant.

Figure 8 shows the $J(V)$ characteristics at room temperature for device thicknesses of 20, 30, and 50 nm, as calculated using the method described in Ref. 39. There are no injection barriers at either electrode, so that the current is space-charge limited and the effect of mirror charges at the electrodes is negligible. It follows from this figure that field-induced detrapping can be very relevant. An increase in the current density of up to half an order of magnitude is obtained at voltages (indicated by the vertical arrows) corresponding approximately to the maximum realistic field mentioned above. Figures 7 and 8 show that field-induced detrapping should be taken into account when the average field in the device $V/L \gtrsim \sigma/ea$. This is comparable to the value above which the mobility in the host shows a significant field dependence.[18] As a rule of thumb we thus conclude that *field-induced detrapping becomes important when the*
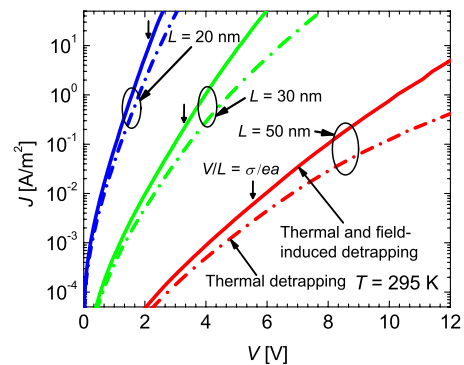

FIG. 8. (Color online) Room-temperature current density vs voltage characteristics for a single-layer single-carrier device with various thicknesses L of the host-guest system described in Sec. IV. The dashed-dotted lines are the model results with thermal detrapping only while for the solid lines also field-induced detrapping (FID) is taken into account. The vertical arrows indicate the voltage values in each device where the average field in the device V/L is equal to σ/ea=0.11 V/nm.

dependence of the mobility on the electric field in the host becomes important.

V. SUMMARY, CONCLUSIONS, AND OUTLOOK

We have shown how the Hoesterey-Letson model for describing the mobility in host-guest systems in the limit of zero electric field may be generalized to the case of finite electric fields. Furthermore, we have developed an easy-to-use method for calculating the mobility in an organic semiconducting host-guest system with a Gaussian host DOS and a general shape of the guest DOS. The model is applicable when the guest concentration is sufficiently small, so that no guest-to-guest hopping occurs. We have demonstrated that, as in the standard Hoesterey-Letson model, also at finite fields the mobility may be viewed as being due to the fraction of charge carriers, the free carriers that are detrapped from the guest sites and reside on the host sites. We have shown that by using a practical parameterization scheme, which provides this field-dependent fraction of free charge carriers, and by using the known field dependence of the mobility in the pure host system, the field dependence of the mobility in host-guest systems may be efficiently calculated. Within the parameterization scheme, the free charge-carrier density is calculated using a generalized field-dependent Fermi-Dirac function.

The field dependence of the mobility in host-guest systems is a combination of the intrinsic field dependence of the mobility of the host material and field-induced detrapping. We have shown that field-induced detrapping becomes quite relevant for fields at which also the intrinsic field dependence of the mobility in the host becomes relevant. Application of the model to typical doped single-layer single-carrier model devices has revealed that under realistic experimental conditions the effect of field-induced detrapping on the current density can be significant. We infer from the analysis that the effect is also relevant in (double-carrier) OLEDs and foresee that our model can be readily combined with existing software for OLED device simulations, making it possible to study the effects of (emissive) dopants in these devices with enhanced accuracy.

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[34] We follow the tradition to use the term "Fermi energy" also at finite temperature, where "chemical potential" would actually be more appropriate.

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