EFFECTS OF CONCENTRATION AND LOCALIZATION LENGTH ON CHARGE CARRIER MOBILITY IN ORGANIC DISORDERED SEMICONDUCTORS

A PROJECT SUBMITTED TO THE DEPARTMENT OF PHYSICS
IN PARTIAL FULFILLMENT OF REQUIREMENT FOR THE
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AT
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By: Seid Melaku

Advisor: Dr. Lemi Demeyu

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Abstract

Using computer simulations, we show that the dependence of the hopping carrier mobility on the electric field $\mu(F)$ in a disordered organic semiconducting polymer of random energy sites described by a Gaussian density of states is determined by the localization length α and not by the concentration of sites N. This result is in drastic contrast to what is usually assumed in the literature for a theoretical description of experimental data and for device modeling, where $N^{-1/3}$ is considered as the decisive length scale for $\mu(F)$. In the proposed it is assumed that the localized states are randomly distributed in energy and space coordinates. The expression for hopping conductivity is obtained for the Gaussian density of states and the analysis of electric field dependent hopping mobility is shown by the Poole-Frenkel behavior is only valid in medium electric field.

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Abbreviations and Symbols

HOMO	the highest occupied molecular orbital
LUMO	the lowest unoccupied molecular orbital
DOS	density of states
ODS	organic disordered semiconductors
GDM	Gaussian disorder model
TOF	time of flight
VRF	variable range of hopping
α	localization length
N	site concentration
ε_F	Fermi level of system
n	total charge concentration
$\varepsilon_i \ and \ \varepsilon_j$	site energies
r_{ij}	separation distance
ν_0	attempt to escape frequency
σ	conductivity
$\langle v \rangle$	drift velocity
F	electric field
D	diffusion coefficient
$\langle r \rangle$	average transition
CV	current-voltage
C_n	critical concentration
τ	relaxation time
ε_∞	equilibration energy
ε_t	transport energy
$\langle t \rangle$	average time step
$\Delta\varepsilon$	activation energy
μ	drift velocity
$\mu(F)$	field dependent mobility
N_p	number of particles

Chapter 1

Hopping Mobility Transport

1.1 Introduction

Organic semiconductors attract currently much attention in scientific community as materials desired for application in modern electronics. The term organic semiconductors covers a large class of materials with a broad variety of properties. Organic semiconductors can be fabricated in crystalline form, as for instance, pentacene and ruberene [1]. The energy spectrum in such materials has classical band structure with charge carriers moving as free particles or polarons in the conduction and valence band. The main focus in this research is on organic disordered semiconductors (ODS), such as polymers and low-molecular weight systems [2, 21]. The interest in ODS is caused by their optoelectronic features and by easy manufacturing, as compared with organic crystals. In contrary to crystalline materials, ODS, possesses neither structural regularity nor spatially extended electron states. Instead, electronic states in ODS are spatially localized [2, 21]. This happens because the overlap integrals for weak Van-der wales interactions between neighboring structural units (molecular or complexes) in ODS's are much smaller than the energy scales of disorder which prevents the formation of extended electronic states [2, 4]. Therefore, charge transfer in ODS due to incoherent tunneling (hopping) of charge carriers between localized states that are randomly distributed in space [2, 21].

Amorphous organic semiconductors are key ingredients for wide variety of optoelectronic devices, such as organic solar cells [8, 11], amorphous organic light emitting diodes[8, 11], laser printers [8, 11] and detectors used in imaging application [8, 11]. Although many day-to-day applications of such materials exist already, the interest grows constantly and new applications hit the market [8, 18] very frequently. The reason for this success is the great flexibility and tune ability (mobility) of organic compounds along with a simple and cost efficient manufacturing process, as compared to crystalline semiconductor nano devices.

In this project (research) the effect of concentration and *localization length* on charge carrier mobility in organic disordered semiconductors is presented and the results are verified by Montecarlo simulatio. In the next sections of this chapter charge Transport model and important systems like *localization length*, *density of states*, *hopping conductivity* and *variable range of hopping* (VRH) are briefly described.

1.2 Localized States

There are two different kinds of disordered semiconductors: Inorganic and organic semiconductors. In each of them atomic or molecular structure is completely disordered. Due to this lack of periodicity, the famous Bloch theorem, that sets the foundation for the crystalline semiconductor physics, is not applicable.

Inorganic amorphous semiconductors consist in most cases of only one or two different types of atoms. Famous examples are pure and hydrogenated amorphous silicon ($a-Si, a-Si:H$) and amorphous carbon ($a-C$). The electronic states in the conduction and valence bands are therefore delocalized. This allows some of the concepts from crystalline semiconductor physics to be applied also for inorganic amorphous materials. However, in the band gap between valence and conduction band, some *localized states* exist in which charge carriers can be trapped.

Organic amorphous semiconductors are carbon-based materials, that consist of larger molecules with conjugated carbon chains as a key feature. The carbon atoms have four electrons in the outer shell (ground state: $1s^2 2s^2 2p^2$) and in organic semiconductors the s and p orbitals hybridize to three sp^2 orbitals. These orbitals result in strongly bound σ bonds. The forth orbital is a p_z orbital perpendicular to the carbon plane formed by σ bonds. The overlap of the p_z electrons from different carbon atoms results in a delocalized band of π orbitals. In this band, both bonding and anti-bonding π and $\pi*$ orbitals exist, *the highest occupied molecular orbital* (**HOMO**) and *the lowest unoccupied molecular orbital* (**LUMO**), respectively.

In the bulk of a disordered organic semiconductor, these π orbitals provide localized electronic states, in the case of an under occupation. This is depicted in Figure 1.1. These localized states are often referred to as *sites*. Their

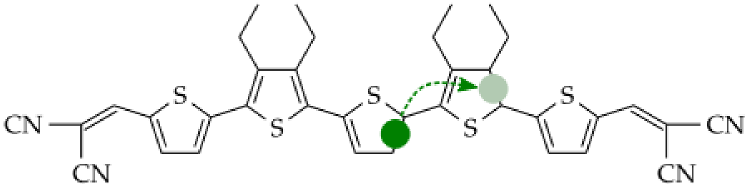

Figure 1.1: Structure of a DCV5T-ethyl molecule, a typical organic semiconductor. Carriers (dark green circle) can tunnel between the under occupied p_z orbitals (light green circle) of the carbon rings.

electronic wave function is localized in space within a certain volume and can therefore be assigned spatial coordinates. The extent of the localization is described by the*localization length* α.

Each of the sites, that can be occupied a charge carrier, has some binding energy. In disordered material energies are different from site to site. The distribution of the sites in space and energy is called the *density of states*, which is important for the description of charge carriers conduction in the the materials.

It is usually assumed that each site may be occupied by only one charge carrier at a time, leaving it in only two possible states, occupied or empty. Charge transport can occur only if the carriers are able to make transitions between the sites. Movement of charge carriers therefore consists of a sequence of trapping and releasing of charge carriers by localized states. This behavior is shown schematically in Figure 1.2. Such a transition from one site to another site is called *hopping*. A sequence of hopping is hence called *hopping conduction (transport)*.

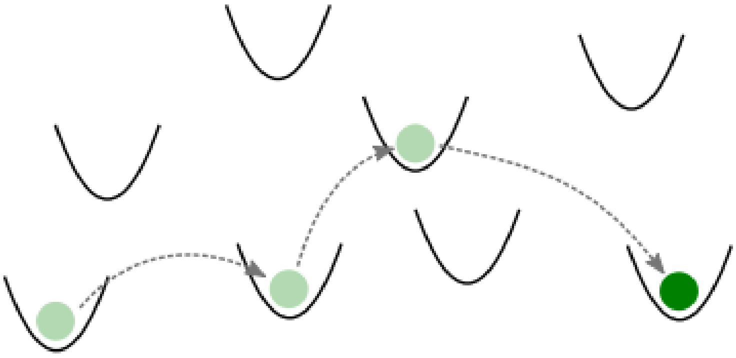

Figure 1.2: Charge carriers are trapped and released from localized states. Due to the different energies of the states, the carriers move in space and energy from site to site. A sequence of such transitions forms charge transport.

Table 1.1: System parameters of some example organic disordered semiconductors.

Material	$\alpha[nm]$	$N[cm^{-3}]$	$N\alpha^3$	Reference
P3HT	0.16	3×10^{20}	0.00123	[2, 3]
$OC_1C_{10} - PP\mathrm{V}$	0.14	3×10^{20}	0.00082	[2, 3]
5T	0.48	5×10^{21}	0.553	[4]

1.3 The localization length

The wave functions of the confined electrons or holes in the localized states are usually assumed spherical or point-shaped. The electron is delocalized within a radius α around a site, this radius is called the *localization radius* or *localization length*. This localization radius strongly depends on the material. While an amorphous inorganic semiconductor may consist of randomly placed single atoms (resulting in a very small localization length), the localized site may be a segment of an organic conducting polymer, and spread over large parts of the molecules.

The second parameter that is related to the localized states is their spatial concentration N. It is convenient to describe both the localization length α and the site concentration N (with one (in three dimensions) dimensionless parameter $N\alpha^3$).

In Table 1.1 some materials with the corresponding values of α, N and $N\alpha^3$ are listed. It is evident from the values that both the site concentration N and the localization length α can vary by orders of magnitude between the materials, which makes the parameter range very broad.

1.3.1 The energy distribution of charge carriers

There is another energy distribution despite the DOS that is important for charge transport related physics in organic semiconductors: The charge carrier distribution. While the spatial concentration of electronic states N is fixed in a solid state material, the concentration of charge carriers n can vary in experiments and applications. We mainly distinguish between two different cases:

In the empty system, the ratio n/N is so small that the carriers are completely independent from each other: A charge carrier that moves through the system will not be hindered by states that are already occupied by other carriers. In this case, we can imagine a single charge carrier in an otherwise empty system and the carrier concentration can be neglected.

However, when the system is filled with carriers, their concentration n must be taken into account. In this case we speak of finite charge carrier concentrations. It depends on the system parameters, at which relative concentrations n/N it is reached, but in some applications, e.g. in field-effect transistors, this case applies. In order to find generally applicable theories, the dependence on the electron concentration n should therefore be taken into account in calculations.

Like in many other physical systems, the electrons or holes, both fermions, follow the Fermi statistics and in thermal equilibrium, the charge carriers are distributed according to the *Fermi-Dirac distribution*

$$f(\varepsilon, \varepsilon_F) = \left[\exp(\frac{\varepsilon - \varepsilon_F}{kT}) + 1)\right]^{-1} \tag{1.1}$$

In Equation (1.2), kT is the thermal energy and ε_F is the *Fermi energy* of the system. It is defined as that particular energy, up to which the electronic states of the system are occupied by charge carriers in the case $T = 0$. The Fermi level is sometimes referred to as the *chemical potential* in the chemical literature. The density of states, the Fermi distribution and the occupation of localized states is shown in Figure 1.3.

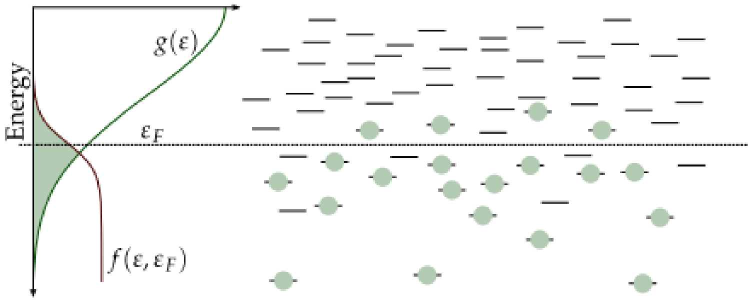

Figure 1.3: The density of states $g(\varepsilon)$ and the Fermi-Dirac distribution of charge carriers $f(\varepsilon, \varepsilon_F)$. Sites up to the Fermi level are occupied with charge carriers (light green circles) while most sites above are empty. The transition between free and occupied sites is measured out at finite temperatures $T > 0$.

When the Fermi level lies very deep as compared to the important energy range, i.e. in the case of an empty system, the exponent of $\exp(\varepsilon\varepsilon_F-)/kT)$ in Equation (1.2) is very large compared to 1. Therefore,

$$\exp\left(\frac{\varepsilon - \varepsilon_F}{kT}\right) + 1 \approx \exp(\frac{\varepsilon - \varepsilon_F}{kT}) \tag{1.2}$$

and Equation (1.2) can be written as

$$f(\varepsilon, \varepsilon_F) \approx \exp(\frac{\varepsilon - \varepsilon_F}{kT}) \tag{1.3}$$

In the so-called *Boltzmann approximation*, the Fermi distribution becomes the *Boltzmann distribution*. This is a useful approximation, that we use very frequently in this work to simplify mathematical calculations. Physically, it means that at energies high above the Fermi level, the charge carrier concentration decays exponentially with lower binding energies.

Since the charge carrier distribution $f(\varepsilon, \varepsilon_F)$ can be interpreted as the probability distribution of finding sites at energy ε occupied by charge carriers, the total number of charge carrier can be calculated with the integral

$$n = \int_0^\infty g(\varepsilon) f(\varepsilon, \varepsilon_F) d\varepsilon \tag{1.4}$$

where n is the number of charge carriers and N is the number of sites per unit volume (usually per cm^3). In our model framework, we always express the carrier concentration n in terms of the site concentration N.

1.4 Hopping Conduction (Transport)

Charge transport in disordered semiconductors consists of a sequence of incoherent tunneling transitions between localized states, called *hopping*. Hopping transport was first studied by Allen Miller and Elihu Abraham in 1960 [6]. Neville Francis Mott later described the variable range hopping model (see Section 1.4.2) in 1968 [7] and was awarded the Nobel Prize for contributions to the theory of charge transport in disordered solids. Since then, these results are applied very successfully to a wide range of theoretical problems in the field of disordered and doped semiconductors. A single hopping transition is depicted in Figure 1.4. For the purpose of finding transport properties like the mobility or diffusivity of charge carriers, one is mostly interested in the transition rates of the hops. While numerous models were developed to describe these rates, by far the most successful one was suggested by Miller and Abraham [6]. The *Miller-Abraham's expression* gives the hopping rate as

$$\nu_{ij} = \nu_0 \exp(-2r_{ij}/\alpha) \begin{cases} 1 & if\ \varepsilon_j \leq \varepsilon_i \\ \exp[-(\varepsilon_j - \varepsilon_i)/kT] & \text{otherwise} \end{cases} \tag{1.5}$$

Equation (1.5) describes the tunneling transition rate from two sites i to j that are separated by the distance r_{ij} and the energies ε_i and ε_j. When the charge carrier relaxes downwards in energy, a phonon is emitted.

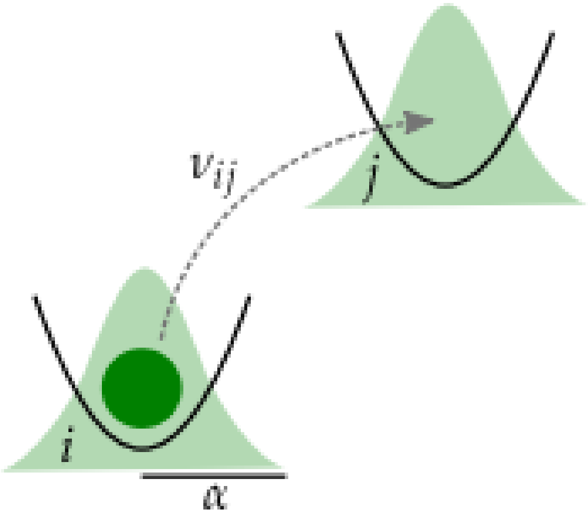

Figure 1.4: A single incoherent tunneling transition or hop between two localized states i and j with the energies ε_i and ε_j. The sites are separated by the distance r_{ij}. a is the localization length of the sites' wave functions. Transitions between the sites happen at a rate of ν_{ij}.

In the case of an activated transition, the required energy is taken up by the absorption of a phonon. ν_0 is the attempt-to-escape frequency and is typically of the order of $10^{12}s^{-1} - 10^{14}s^{-1}$.

Equation (1.5) consists of two exponentially decaying factors. The first one is the tunneling part of the rates and accounts for the distance between the sites that take part in the transition. The localization length α (see Section 1.3) is assumed equal for both sites. It describes the inverse of decay constants of the localized wave functions. It is evident that far hops and small localization radii lower the hopping frequency ν while hops between sites, that are very close and have large α, are very fast.

The second exponential function in Equation (1.5) accounts for the energy difference between the sites. It is the Boltzmann weight for thermal activation and can be interpreted as the probability to pick up a phonon with the corresponding energy.

It is important to note that in a transition between two sites i and j, the hop from the site higher in energy to the lower one is always faster than a hop in the opposite direction. Since only hops upwards in energy are temperature dependent, the temperature of the system (expressed in kT) is closely related to the frequency of activated hops. Thus, it influences the path of the charge carrier in the energy landscape during hopping transport. It is the interplay between these two exponential functions in Equation (1.5), that is responsible for many interesting transport characteristics in disordered organic and inorganic semiconductors.

1.5 Charge Carrier Mobility and Diffusivity

In applications of semiconducting materials, the most important characteristic is in many cases the charge carrier mobility μ. It is closely related to the conductivity ($\sigma = \mu ne$) and resistivity ($\rho = \sigma^{-1}$) of the material. It describes the drift velocity $\langle v \rangle$ of the carriers as a response to an external electric field F:

$$\mu = \langle v \rangle / F \tag{1.6}$$

A charge carrier motion (hopping) in a disordered system resembles a Brownian motion like behavior. It makes random transitions of a certain length in space and for each of these transitions, a certain time is needed a *diffusion coefficient* D for one dimensional motion as

$$\langle r \rangle = \sqrt{2D\langle t \rangle} \tag{1.7}$$

with $\langle r \rangle$ and $\langle t \rangle$ being the average transition distance and time respectively.

The drift mobility μ and diffusion coefficient D are related via a simple law, the *Einstein relation* [1, 8]:

$$\mu / D = e / kT \tag{1.8}$$

Equation (1.8) is valid in a wide variety of systems and also applicable for hopping conduction in amorphous semiconductors within a broad parameter range [1, 8].

1.6 Transport Modes

In the previous sections, the material structure and parameters were introduced and the single hopping transitions explained and mathematically described. A sequence of these single transitions forms charge transport. While the path of a charge carrier in the spatial dimensions is, apart from fluctuations, simply defined by the direction of the electric field, the behavior in the energy landscape is much more complicated. Since differences in energies make a huge contribution to the hopping rates, as described in Section 1.3, and therefore influence decisively the charge carrier mobility, the energetic part of the path of the carrier is very important and needs to be studied thoroughly.

1.6.1 Dispersive Transport

In the *dispersive transport* regime, charge carriers are slowed down during conduction. This happens only as long as the charge carrier distribution is not in thermal equilibrium. In this regime, the charge carriers are usually trapped in energetically deeper and deeper states and have to perform longer and longer tunneling transitions to hop to the next destination site. As the hopping rates decay exponentially with increasing distances, the average speed of the charge carrier is reduced over time.

Since the mobility of charge carriers during dispersive transport depends on time and therefore, e.g. in time-of-flight (TOF) experiments, on the sample length, it is an experimentally accessible quantity. The dispersive transport can therefore be used to study system characteristics.

1.6.2 Variable-Range Hopping

The *variable range hopping* (VRH) was suggested by Neville Mott [6, 19]. Mott assumed a constant density of states and low temperatures. In his case, all transport happens within an energy range $\Delta\varepsilon$ around the Fermi energy ε_F. Applying the criterion, that within this energy range $\Delta\varepsilon$ and a hopping distance of r, there must be exactly one reachable destination site, Mott found the famous *Mott law* for the conductivity in the system:

$$\sigma = \sigma_0 \exp[-(\frac{\mathrm{T_0}}{\mathrm{T}})^{1/4}] \tag{1.9}$$

$$\mathrm{kT_0} = \frac{\beta}{\mathrm{g}(\varepsilon_\mathrm{F})\alpha^3} \tag{1.10}$$

Here, α is the localization length, $g(\varepsilon_F)$ the DOS at the Fermi energy and β is some parameter that lies, according to different theories, in the range 10.0 to 37.8.

The variable range hopping is closely connected with the Miller-Abraham's hopping rates, Equation (1.5). As long as a carrier can find shallow and unoccupied sites with energies below its current state, it will perform a *nearest neighbor hopping* to energetically lower sites, since in this case the rates are only limited by the spatial tunneling distances. However, at some point the next unoccupied site with deeper energy might be so far away, that it is faster for the carrier to perform an activated hop upward in energy. These activated hops resemble the variable range hopping.

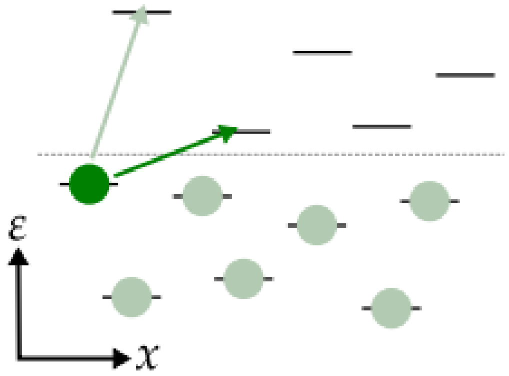

Figure 1.5: Mott's variable range hopping model (VRH). A charge carrier (dark green circle) might choose a site far in space (dark green arrow) over the nearest neighbor (light green arrow), when the energy difference to the latter is too high.

In such transitions, the carrier essentially optimizes the hopping difficulty

$$A(\varepsilon_i, \varepsilon_j, r_{ij}) = \frac{2r_{ij}}{\alpha} + \frac{\varepsilon_i - \varepsilon_j}{kT} = \ln(v_0/v_{ij}) \tag{1.11}$$

It might therefore choose a very distant site over the nearest neighbor, given the energetic difference is much lower. This situation is shown in Figure 1.5.

1.6.3 Multiple Trapping Model

The *multiple trapping model* describes a transport mode, in which conduction is assumed to happen at or above a certain energy only. In amorphous inorganic semiconductors, this energy threshold is called *mobility edge*. Charge carriers are trapped by localized states and released again with an activated hop to the mobility edge. Above this edge, the electronic states are extended and the mobility is therefore orders of magnitude higher than during variable range hopping (VRH). This is why the conduction occurs only within these extended states. Multiple trapping is shown in Figure 1.6. At very low temperatures, the multiple trapping transport in inorganic semiconductors migrates to variable range hopping explained in Section 1.6.2.

Multiple trapping also occurs in amorphous organic semiconductors, except that the mobility edge is replace by the transport energy level. Carriers are activated to the transport energy and since these hops contribute the most to transport coefficients like the mobility, the analogy to the mobility edge is justified.

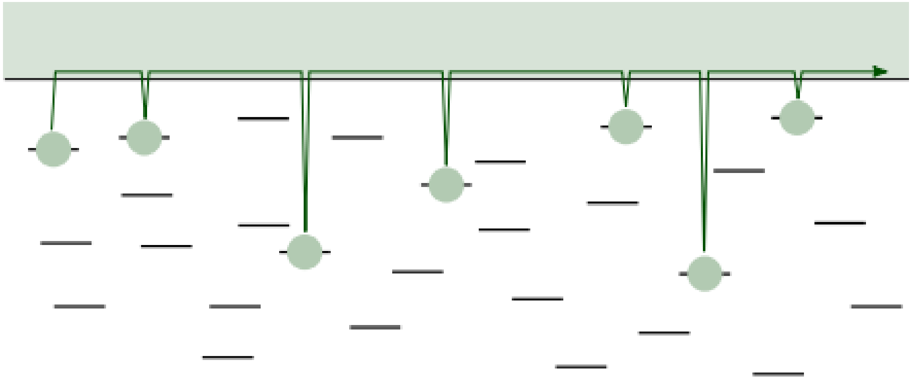

Figure 1.6: Multiple trapping transport. The charge carrier (light green circles) is trapped and released into and from localized states (black lines). Conduction happens above the mobility-edge (light green area).

1.6.4 Nearest Neighbor Hopping

The nearest neighbor hopping describes a hopping regime, in which the tunneling part of the hopping rates in Equation (1.6) is so much slower than the energy contribution, that only the nearest neighbors are addressed in hops. This is the case for very high temperatures or very small localization radii α.

Even though a random site distribution is the defining property of disordered semiconductors, these can in some limits be modeled using a lattice structure and keeping only the energy disorder. In such lattice models, the transition from nearest neighbor hopping to variable range hopping (Section 1.6.2) can be studied.

Chapter 2

Charge Carrier Mobility Variation With Concentration and the Density of States (DOS)

The density of states (DOS) is describes the spatial and energetic distribution of localized states and influences mobility variation decisively. Not only in the field of disordered semiconductors is the knowledge of DOS very important for theoretical calculations. In organic materials, this distribution function is still one of the most searched-for properties. While its shape is known for inorganic amorphous semiconductors, there is an ongoing dispute in the scientific community whether the exponential DOS can be applied to organics as well [10]. Each year appear numerous publications, that utilize some DOS function without discussing and justifying the choice.

In this chapter, we find that only close to Gaussian DOS functions can explain experimental results obtained for two of the most widely studied organic semiconductors.

2.1 Experiments

Experiments, in which the dependence of the charge carrier mobility μ on carrier concentration n was measured, show that in organic materials the mobility becomes constant at low concentrations. While this is one of the rare publication with direct $\mu(n)$ results, such observations can be derived from common current-voltage (CV) measurements [12]. Numerous experimental studies show the concentration independent mobility at low n for amorphous organic semiconductors. [2, 13-15]

This observation strongly contradicts the dispersive transport behavior, which is a direct consequence of the exponential density of states. For this reason we can already now exclude the purely exponential shape of the density of states from the possible DOS functions in organics!

Some materials in which a constant mobility at low carrier concentrations can be derived from CV measurements are gathered .

2.2 How to Find out the Density of States

In the previous section, it was shown that numerous disordered organic semiconductors show a concentration independent mobility at low charge carrier concentrations. In the purely exponential density of states, concentration limited dispersive transport is expected, hence $\mu = \mu(n)$ at all carrier concentrations n. This contradicts the situation observed in experiments and rules out the exponential DOS as a candidate for organic disordered materials.

While this result is already very important, the question of the shape of the DOS still persists. It is answered in the following sections. We assume a set of trial DOS functions

$$g(\varepsilon) = C\frac{N}{\sigma}\exp[-(\frac{\varepsilon}{\sigma})^p] \tag{2.1}$$

In Equation (2.1), N is again the total concentration of localized states, C is the normalization factor and σ is the width of the DOS or the disorder strength. In further calculations, we will use the dimensionless parameter σ/kT to describe this quantity. p is the exponent of the DOS and is varied between 1.0 to 2.2. This includes the purely exponential shape, $p = 1$, $C = 1$, known from inorganic disordered semiconductors, as well as a Gaussian shape, $p = 2$, $C = \sqrt{\pi}/2$.

For non-integer p-values, the DOS for energies $\varepsilon < 0$ is not well defined, which is why we use the convention $\varepsilon \geq 0$ everywhere. This effects the transport coefficients only at extremely high fillings or temperatures.

2.2.1 The Gaussian DOS

Before the general properties of density of states functions, that decay steeper than exponentially, are analyzed, the Gaussian shape and its history shall be explained briefly.

In 1981, Heinz Bässler [17] suggested a Gaussian shape of the density of states in organic solids:

$$g(\varepsilon) = \frac{N}{\sqrt{2\pi}\sigma} \exp[\frac{-\varepsilon^2}{2\sigma^2}] \tag{2.2}$$

His argumentation was based on polarization fluctuations via a normal distribution. Bässler later published a Review in which these arguments are strengthened and some consequences of the Gaussian DOS are derived. [17]

It is worth mentioning that the assumption of a Gaussian DOS and many of Bässler's results proved to be correct. Although more and more researchers became convinced of the idea of a Gaussian shape of the DOS, in the majority of publications a purely exponential form is still assumed. This is for the following reasons.

Bässler himself claimed that analytic solutions of the hopping transport problem are not possible in the Gaussian density of states [17]. This belief and the fact, that the exponential DOS is much better understood than the Gaussian, leads researchers to stick to the well-known purely exponential density of states from amorphous inorganic semiconductors.

The second reason for the popularity of the exponential DOS in organics is that Vissenberg and Matters claim in one of the first and most cited theoretical articles [18] on amorphous organic semiconductors, that the Gaussian and exponential DOS essentially are the same and it is therefore sufficient to use the exponential shape.

2.2.2 Equilibration Energy

To understand the most important difference between the purely exponential DOS ($p = 1$ in Equation (2.1)) and one that decays steeper ($p > 1$), the equilibration energy must be introduced.

In thermal equilibrium, charge carriers are distributed via the Fermi-Dirac distribution $f(\varepsilon, \varepsilon_F)$ (Equation (1.2)). This function can be interpreted as the probability to find a state at a certain energy ε occupied. The energy distribution of the charge carriers in the system is therefore described by the product of the density of states $g(\varepsilon)$ and the Fermi function $f(\varepsilon, \varepsilon_F)$:

$$g(\varepsilon)f(\varepsilon, \varepsilon_F) = C\frac{N}{\sigma} \exp(-(\frac{\varepsilon}{\sigma})^p)[\exp(\frac{\varepsilon_F - \varepsilon}{kT}) + 1]^{-1} \tag{2.3}$$

This distribution has one very interesting property: In the case $p > 1$, it has a maximum value and converges to zero for $\varepsilon \rightarrow \pm\infty$, whereas it diverges in the case $p = 1$. This means the following.

In the exponential density of states, $p = 1$, the majority of the charge carriers in the system occupy states at and below the Fermi level. In the case $p > 1$ the carrier distribution still depends on the Fermi level, but the carriers spend most of their time at an energy ε_∞ independent from ε_F. This energy ε_∞ can be calculated as follows.

Let us assume a system with $p > 1$, with such a small amount of charge carriers, that the Fermi level always lies much deeper than the peak of the carrier distribution $g(\varepsilon)f(\varepsilon, \varepsilon_F)$. In this case, the Fermi distribution can be approximated by the Boltzmann function (Equation (1.4)), as shown in Section 1.2.3. The product $g(\varepsilon)f(\varepsilon, \varepsilon_F)$ becomes

$$g(\varepsilon)f(\varepsilon, \varepsilon_F) \approx g(\varepsilon)\exp(\frac{\varepsilon}{kT})\exp(-\frac{\varepsilon_F}{kT}) \tag{2.4}$$

The dependence on the Fermi level in Equation (2.4) is just a scaling factor and can be dropped, when one is only interested in the energy position of the carrier distribution peak. $g(\varepsilon)\exp(\frac{\varepsilon}{kT})$ has a maximum at the following position, which can easily be calculated analytically:

$$\varepsilon_\infty = \sigma(\frac{\sigma}{kT}\frac{1}{p})^{\frac{1}{p-1}} \tag{2.5}$$

The energy $\varepsilon_\infty$is called *equilibration energy* [17]. It is the maximum of the charge carrier distribution, to which the DOS $g(\varepsilon)$ and the Fermi distribution $f(\varepsilon, \varepsilon_F)$ contribute. (As stated before, the carrier distribution does not have a maximum in the case $p = 1$, which is the essential difference to the cases with $p > 1$)

Note that ε_∞ is usually defined not as the maximum but the average value of the distribution $g(\varepsilon)\exp(\varepsilon/kT)$. It is therefore calculated properly via

$$\langle\varepsilon_\infty\rangle = \frac{\int_0^\infty \varepsilon g(\varepsilon)\exp(\varepsilon/kT)}{\int_0^\infty g(\varepsilon)\exp(\varepsilon/kT)} = \frac{-\sigma^2}{kT} \tag{2.6}$$

However, in the range of parameters we study, Equation (2.5) and Equation (2.6) are close enough to justify the usage of the former. Equation (2.8) is not solvable analytically for non-integer p values.

The most important consequence of this carrier distribution is, that the position of the equlibration energy ε_∞ is concentration independent! Under the assumption, that the Boltzmann approximation holds and $p > 1$, the charge mobility should therefore also be independent of the charge carrier concentration n. This is exactly the same observation made in the experiments described in Section 2.1.

The concentration independent mobility therefore evidence that in disordered organic materials the DOS must decay steeper than purely exponentially. In the following sections, the parameter space of allowed p values is reduced further and the results are compared to experimental data.

2.2.3 Charge Carrier Relaxation

In order to restrict the possible values of p further, we need to study the relaxation of charge carriers in our system. The charge relaxation process resembles the multiple trapping mode (see Section 1.6.3), except that in this case the role of the mobility edge is taken over by a particular energy ε_t, at which conduction happens. This energy is called the *transport energy*.

In non-equilibrium conditions, charge carriers in the system perform dispersive transport as explained in Section 1.6.1. They find deeper and deeper states and the mobility slows down in the course of time. However, in the case for $p > 1$, this stops as soon as they reach the equilibration energy. The time that is needed for the charge carriers to equilibrate, is called the relaxation time τ. A successful model to calculate τ, is to use the time of the longest (and final) activation process during the relaxation. Since carriers that arrive at or below ε_∞ are assumed in thermal equilibrium, this final energy is exactly ε_∞. The relaxation time is therefore described by

$$\tau = 1/v(\varepsilon_\infty, \varepsilon_t) = v_o^{-1} \exp(2R(\varepsilon_t)/\alpha) \exp(\frac{\varepsilon_\infty - \varepsilon_t}{kT}) \tag{2.7}$$

Equation (2.7) is the inverse Miller-Abraham's hopping rate for an activated hopping process between the equilibration energy ε_∞ and the transport energy ε_t. $R(\varepsilon_t)$ is assumed to be the average distance between localized states with energies around ε_t. Since the tunneling factor $\exp(2R(\varepsilon_t/\alpha)$ is always larger than unity and we are only interested in the lower bound of the relaxation time, we neglect this factor. We will also assume $\varepsilon_t = 0$. We end up with the following expression for the relaxation time:

$$\tau = v_o^{-1} \exp(\frac{\varepsilon_\infty}{kT}) \tag{2.8}$$

When a constant mobility is observed in experiments, the relaxation process cannot play an important role for charge transport. It must therefore be much shorter than the time, that a single charge carrier needs to traverse through the sample. Otherwise, the time dependent dispersive transport would be mirrored in the measured results.

Let us now estimate, based on Equation (2.8), the values of ε_∞ and the relaxation times τ for different disorder strengths σ/kT and DOS exponents p.

Equation (2.5) is plotted for different parameters in Figure 2.1. The right-hand y-axis shows some corresponding relaxation times according to Equation (2.8). The parameter ν_0, the attempt-to-escape frequency, is chosen as $\nu_0 \approx 10^{12}s^{-1}$ which is a reasonable choice.

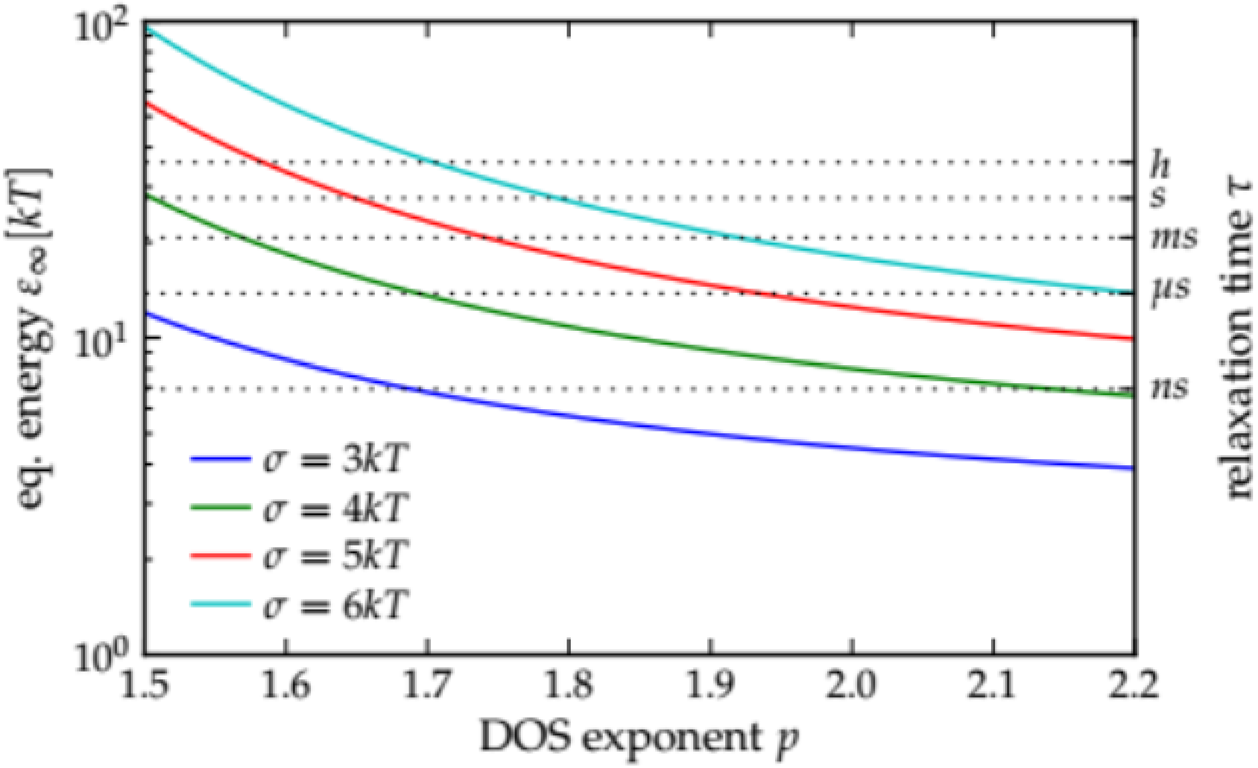

Figure 2.1: The equilibration energy ε_∞ versus the density of states exponent p for different values of σ/kT. On the right axis, the time scale of the corresponding relaxation times τ is shown.

A typical time-of-flight experiment to measure the mobility is finished within microseconds. It is therefore clear from the figure, that for p values of $p < 1.5$ the relaxation times would be far too long to explain the experimentally observed concentration independent mobility. This allows us to restrict the range of allowed p values to $p \geq 1.5$.

2.2.4 Concentration Dependence of the Charge Carrier Mobility

The determination of the allowed p-range for the trial DOS functions of Equation (2.1) in the previous sections is a rather qualitative one: By estimating the expected relaxation time of the charge carriers, the values for $p < 1.5$ are ruled out. To find a more accurate estimation of p in a particular material, one must study the concentration dependence of the mobility.

As explained in Section 2.2.2, charge carriers in organic semiconductors spend most of their time in states with energies in the vicinity of the equilibration energy ε_∞. As long as the Fermi level lies far below this energy, the charge carrier mobility appears concentration independent.

However, when the system is filled with electrons or holes, the Fermi level ε_F climbs higher and higher until it reaches ε_∞. This happens at a critical concentration of charge carriers, n_c. At this concentration, the Fermi level takes over the role of ε_∞: It then becomes the lower bound of the activation processes that fix charge transport properties. Since ε_F depends on the concentration n, charge carrier mobility must now appear concentration dependent.

We can therefore formulate the following criterion for the critical concentration n_c, above which charge carrier mobility should appear concentration dependent:

$$\varepsilon_F(n_c) \approx \varepsilon_\infty \tag{2.9}$$

The concentration of charge carriers in diodes is proportional to the applied voltage. The mobility-concentration data $\mu(n)$ can be extracted from current-voltage (CV) measurements.

However, there are also results of $\mu(n)$ measurements published directly [2]. Especially the data from Tanase *et al.* An example for how to find the DOS exponent p in organics. In Figure 2.1 of this publication the mobilities m in an organic diode (*P3HT*) and field-effect transistor ($OC_1C_{10} - PPV$) are plotted versus the charge carrier concentration n. In both materials, the mobility is constant up to a certain concentration n_c and then starts growing.

Using the criterion in Equation (2.9) and the parameters given by Tanase *et al.*, we can calculate n_c for different values of the DOS exponent p. The results can then be compared to the one obtained from the experiment. Tanase *et al.* specify the following parameter values:

$$N = 3 \times 10^{20} cm^{-3}, \;\; \sigma = 0.112\sqrt{2}eV, \;\; T = 293K, \;\; \alpha = 0.16nm \tag{2.10}$$

With these parameters, we can calculate $\varepsilon_F(n_c)$ via Equation (1.5), ε_F via Equation (2.6) and apply the criterion of Equation (2.9) to find $n_c(p)$. We use three different values of σ to check, whether the results are stable against variation of this parameter. It is apparent from the figure that the DOS exponent p must lie in the range $1.7 < p < 2.2$ to match the experimental data. Only at those p, where the dashed lines, which resemble the experiments, intersect with the results from the theory, an agreement can be reached.

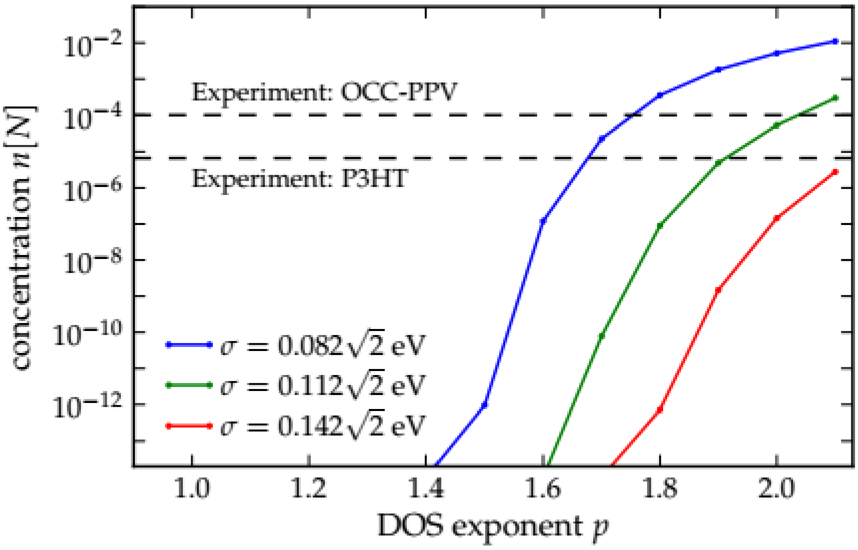

Figure 2.2: The critical concentration n_c above which charge transport appears concentration-dependent versus the exponent of the DOS p. The values obtained from the experiments in References [2 , 3] are indicated as dashed lines. The temperature is $kT = 0.025eV$.

Chapter 3

Localization Length for the Field Dependence Hopping Mobility in Lattice Parameter

In the previous chapters, the theoretical basis for mobility in disordered organic semiconductors is formed. After introduction on microscopic processes involved in hopping mobility transport in Chapter 1, the importance and the role of DOS is illustrated and its shape is determined in Chapter 2. In this chapter, localization length for the field dependence hopping mobility in lattice parameter and localization length affects $\mu(F)$ in lattice model is presented and localization length determines $\mu(F)$. Lastly, it is verified by comparison with computer simulation of mobility.

3.1 Localization Length for the Field Dependence of Hopping Mobility

The most popular theoretical model to describe charge transport in ODSs is the so-called Gaussian disorder model (GDM), according to which localized stales have a Gaussian energy distribution

$$g(\varepsilon) = \frac{N}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right) \tag{3.1}$$

Here σ is the energy state of the spectrum, usually estimated in ODS's to the order of $\sigma \approx 0.1eV$ and N is the concentration of randomly distributed localized states (sites). A typical estimate for the latter parameter is between $N \simeq 10^{20}cm^{-3}$ and $N \simeq 10^{2}cm^{-3}$

The hopping rates are usually assumed to be described by the Miller-Abrahams expression. For each pair of sites i and j, the rate v_{ij} is determined by their energy difference $\varepsilon_j - \varepsilon_i$ and position difference $r_{ij} \equiv r_j - r_i$.

$$v_{ij} = v_0 \exp\left(-\frac{2\left|\mathbf{r}_{ij}\right|}{\alpha}\right) \gamma\left(\varepsilon_j - \varepsilon_i + e\mathbf{F}.\mathbf{r}_{ij}\right) \tag{3.2}$$

with

$$\gamma\left(\Delta\varepsilon\right) = \begin{cases} \exp\left(-\Delta\varepsilon/kT\right), & if\ \Delta\varepsilon > 0, \\ 1, & \text{otherwise}, \end{cases} \tag{3.3}$$

where α is the localization length of charge carriers, F is the electric field, and ν_0 is a prefactor determined by the tunneling mechanism. The localization length α in ODSs is estimated at the order of 10^{-8} cm, which is much smaller than the intersite distance $N^{-1/3}$. Therefore we follow the usual assumption that α can be considered to be independent of the concentration of sites N.

While powerful and transparent analytical theoretical tools have been developed to describe the dependencies of the hopping mobility μ on T, N, α, σ and on the concentration of carriers n, as highlighted in recent reviews theoretical studies of the dependence $\mu(F)$ have mostly been focused on computer simulations. The group of Bässler simulated $\mu(F)$ on a cubic lattice and fitted results in the form of the parameterized equation

$$\mu(F) = \mu_0 \exp\left[-\left(\frac{2}{3}\frac{\sigma}{kT}\right)^2\right] \exp\left\{\tilde{C}\left[\left(\frac{\sigma}{kT}\right)^2 - B\right]\sqrt{F}\right\} \tag{3.4}$$

where μ_0 is a field-independent prefactor.

Two parameters, $\tilde{C}$ and B are involved in this fitting. The parameter $\tilde{C}$ is assumed to depend on the lattice constant b (distance between localization sites) having thevalue $\tilde{C} = 2.9 \times 10^{-4}$ cm$^{1/2}$ for $b = 0.6$ nm. Although simulations were performed on regular cubic grids, a non diagonal disorder has been introduced into simulations by Bässler *el. al.* in order to mimic spatial disorder. The exponent $(2 \mid rij \mid /\alpha$ in Equation 3.2 was rewritten in the form $2\lambda b \mid rij \mid /b$ where b is the lattice spacing, and the parameter λ can he viewed as the inverse localization length. The factor $2\lambda b$ was distributed in a Gaussian manner with the width Σ around the value $2\lambda b = 10$. The parameter B in Equation 3.4 was set equal to $B = 2.25$ for $\Sigma < 1.5$ and to $B = \Sigma^2$ for $\Sigma \geq 1.5$. Equation 3.4 is one of the most frequently used equations in the context of organic semiconductors.

A similar approach to determine $\mu(F)$ was used by Pasveer el al., who reduced the lattice GDM of Bässler *el al.* to the case $\Sigma = 0$ and here with completely eliminated spatial disorder. Calculating numerically $\mu(F)$ in the framework of this GDM on acubic lattice, Pasveer *et.al.* fitted results to the analytical formula

$$\mu(T, n, F) \approx \mu(T, n)\phi(T, F) \tag{3.5}$$

with $\phi(T, F)$ in the form

$$\phi(T, F) = \exp\left\{0.44\left[\left(\frac{\sigma}{kT}\right)^{3/2} - 2.2\right] \times \left[\sqrt{1 + 0.8\left(\frac{F_{eb}}{\sigma}\right)^2} - 1\right]\right\} \tag{3.6}$$

where b is the lattice constant. The latter equations are sometimes considered universal and they are the basis for the commercially available.

Pasveer et. al. mentioned that Equation 3.6 “should merely be considered as a description of the numerical data in a limited parameter range” promising to rationalize this parametrization in future work. We show below that neither Equation 3.4 nor Equation 3.6 can be rationalized because they do not contain decisive parameters responsible for the field-dependent mobility $\mu(F)$. Equations 3.4 and 3.6, which arc used by thousands of researchers, were obtained by fitting the numerically simulated data under the assumption that the decisive parameter for the dependence$\mu(F)$ is the intersite distance, parameter b in Equation 3.6. We rigorously prove below that this assumption is wrong and the intersite distance is irrelevant for the field-dependent mobility in disordered systems. One should instead use the localization length α as the decisive length scale determining the field dependence of the hopping carrier mobility $\mu(F)$. A theoretical recipe on how to describe the dependence $\mu(F)$ in disordered materials will be formulated below, which should encourage researchers to reanalyze their data on $\mu(F)$ in disordered organic semiconductors.

The paper is organized as follows. we first stay for simplicity in the framework of the reduced GDM used by Pasveer el. al. i.e., on a cubic lattice without spatial disorder. We show that already in this oversimplified case, Equation 3.4 and Equation 3.6 are incompatible with each other even if the same material parameters in these equations are used. We further show that the results of computer simulations by Pasveer el. al are incompatible with the results of computer simulations by Bässler el. at. carried out in the framework of the same reduced GDM on the cubic lattice (i.e., for $\Sigma = 0$). Performing our own computer simulations, we prove that the localization length α not even present in Equations 3.4 and 3.6, is responsible for this discrepancy in the simulations and that the localization length affects decisively the field dependence of carrier mobility.

We consider the GDM on spatially random sites, i.e., not anymore on a lattice, and show by computer simulations that the localization length α is the only spatial scale responsible for the field-dependent hopping mobility. Our computer simulations show herewith that the intersite distance, present in the form of lattice constant b in Equation 3.6 is irrelevant for the field-dependent mobility $\mu(F)$.

3.2 Localization Length Affects $\mu(F)$ in the Lattice Model

Before considering a realistic case of a spatially disordered system, let us analyze the simulated data on the field dependent mobility $\mu(F)$ available in the literature which were obtained on regular cubic lattices and served for parametrization by Equations 3.4 and 3.6.

Let us first check the compatibility of Equations 3.4 and 3.6 with each other. In order to enable the comparison, we plot the data of Bässler el. al. for the case $\Sigma = 0$, i.e., with $B = 2.25$, since Pasveer el. al. simulated for $\Sigma = 0$. The value $T = 300K$ was used in simulations by Bässler el. al., which gives $\sigma = 0.075eV$ for $\sigma/kT = 3$. The difference in the dependencies $\mu(F)$ given by Equations 3.4 and 3.6 for the same sets of parameters is striking.

The apparent inability of Equation 3.4 to fit the simulated data evidences the poor accuracy of this equation but it can hardly be considered as an issue of fundamental importance. However, it is surely an issue of fundamental importance to elucidate the difference in the results of the two simulations for the same value $\sigma/kT = 3$ because the difference between the data obtained in simulation by the group of Bässler and byPasveer *et al.* is compatible to the total effect of F on μ.

The apparent difference in the simulated systems lies in the choice of the parameter b/α. While the group of Bässler simulated for $b/\alpha = 5$, Pasveer *el al.* simulated for $b/\alpha = 10$. In order to check the validity of those previous simulations, we earned out simulations on a cubic lattice similar to those carried out by Bässler *et al.* and by Pasveer *et al.* Our data $b/\alpha = 10$ confirm the data by Pasveer *et al.* with $b/\alpha = 10$ and we simulate $Np = 10$ and $Np = 20$, implying that the computer simulations by both were correct. However, it has not been recognized in previous simulations that the shape of the dependence $\mu(F)/\mu(0)$ is sensitive to the choice of b/a.

This result shows that neither Equation 3.4 nor Equation 3.6 can be considered as universal because these equations do not even contain the localization α. Furthermore, this result shows the apparent deficiency of doing physics by computer simulations. Parameterized phenomenological equations, such as Equation 3.4 and Equation 3.6, do not contain the material parameter which is decisive for the field-dependent mobility $\mu(F)$. Being interested in the dependence $\mu(F)$ for realistic spatially disordered systems rather than for cubic grids, we will consider in the rest of this paper a system of sites distributed in space randomly.

3.3 Localization Length Determines $\mu(F)$

In order to discern the decisive length scale (α, $N^{-1/3}$ or some combination of these parameters) for the field dependence of μ in a system of random sites, we performed computer simulations using the standard Monte Carlo procedure. A disordered system is created with $100 \times 100 \times 100$ sites distributed randomly in a box of $D = 100$, so that the average inter-site distance $N^{-1/3}$ is unity. The site energies are chosen randomly according to the DOS given in Equation 3.1. A single electron is placed onto a random site i and in each simulation step performs a hopping transition to another site j with probabilities weighted by hopping rates given by Equation 3.2 and 3.3. After each hop, the system time is advanced by $\tau = v_{ij}^{-1}$. Initially, the electron is allowed to make 5×10^7 relaxation hops to ensure steady-state conditions, after which statistics is collected for 5×10^8 hopping transitions. The simulations were repeated. The realistically chosen parameters were $\sigma/kT = 4$ and $\sigma/kT = 5$.

Chapter 4

Methodology

4.1 Monte Carlo Simulation Techniques

Monte Carlo methods are a broad class of computational algorithms that relay on repeated random sampling to obtain numerical results. Their essential idea is using random numbers to solve problems that might be deterministic in principle. The Monte Carlo Simulation (MCS) was numerical approach to find charge transport properties in disordered semiconductors. It is the most popular and widely used tool in this field of research.

In this work, the effect of localization length on charge carrier mobility on organic disordered semiconductors is studied using Monte Carlo Simulation method. It consider holes and electrons as charge carriers and limit the study to the low charge carrier density in zero field regime, so that the interaction between charge carriers under consideration is neglected.

As soon as a charge carrier performs a hop, the destination position is chosen randomly on the basis of the probabilities of hopping to each possible destination site. The probability of hopping from one position to another is found based on the hopping rate given by Eq. (1.5). The total rate of hopping of all charge carriers is used to randomly choose the carrier dwell time on each site.

The role of the system size on the simulations results is studied in detail and show that in order to get reliable results on the effect of localization length on charge carrier mobility, one need to perform simulations on enormously large systems. During the actual simulations the distance that the charge carriers travel in each direction and the simulation time is stored. So the effect of localization length on variation of charge carrier mobility is evaluated.

4.2 Model of the Simulation

The system is modeled as a simple cubic lattice $L_x \times L_y \times L_z$ sites, where L_x, L_y and L_z denote the size of the lattice in the X,Y and Z directions, respectively, with lattice constants a and energy at each lattice site is ϵ_i chosen randomly according to Eq. (3.4) periodic boundary condition are considered in all the three dimensions, with no applied electric field to the system. Simulation is performed on regularly arranged three dimensional lattice sites, with the assumption that the hopping among the lattice site is governed by the rate equation given by Eq. (1.5). We only consider the situation of uncorrelated energies at different sites. This means that the energy ϵ_i at each site is randomly drawn from Gaussian density of states given by Eq. (2.2). These disordered energies are uncorrelated.

Each simulation step starts with a random distribution of charge carriers (N_p) over the sites, provided that N_p divided by the number of sites (charge carrier density) is low. One site must not be occupied by more than one charge carrier at a time or avoid double occupancy. Since we are mainly interested in charge carrier mobility at very low carrier density, we neglect the effect of electrostatic interactions. Then the number of charge carrier is 100 or $\frac{N_p}{N} = \frac{100}{100\times100\times100a^3}$ over N sites, where a is a lattice parameter which is about $1nm$ for disordered organic semiconductors.

The simulation procedures begin by the formulation of the three dimensional lattice of $100 \times 100 \times 100$ unoccupied sites. The nearest neighboring sites to which each particle can hop is restricted to $3 \times 3 \times 3 - 1 = 26$ only. The number is restricted to 26 because involving more number of possible destinations are computationally expensive. Two random variants are needed to complete a step in the random walk. First, a dwell time τ must be drawn to determine the dwell time of the charge spends at the site before it will to the next. The second random variant is needed to make a transition. Then we solve for the normalized transition probability and make use of a stochastic approach to move the charge around. In each simulation step, select one pair of sites. The probability of hopping a charge carrier at site i to site j is calculated from

$$P_{ij} = \frac{v_{ij}}{\sum_{ij} v_{ij}} \tag{4.1}$$

where $i = 1, 2, 3, ...100$ and $j = 1, 2, 3, ...26$

Here, $\sum$ is done overall possible hops of all the particles and total probabilities are normalized to 1. Each hop corresponds to the physical time or the mean dwelling time τ at site i is given by

$$t_{av} = \frac{1}{\sum_{ij} v_{ij}} \tag{4.2}$$

The exact time is approximated from the relation

$$t = -tav \ln(1 - r) \tag{4.3}$$

where r is a random number taken from a uniform distribution between 0 to 1.

Chapter 5

Results and Discussion

In the previous chapters, the theoretical basis of charge carrier mobility in organic disordered semiconductors is presented. This chapter presents the discussion of results from the Montecarlo simulation on the effects of concentration and localization length on charge carrier mobility in organic disordered semiconductors.

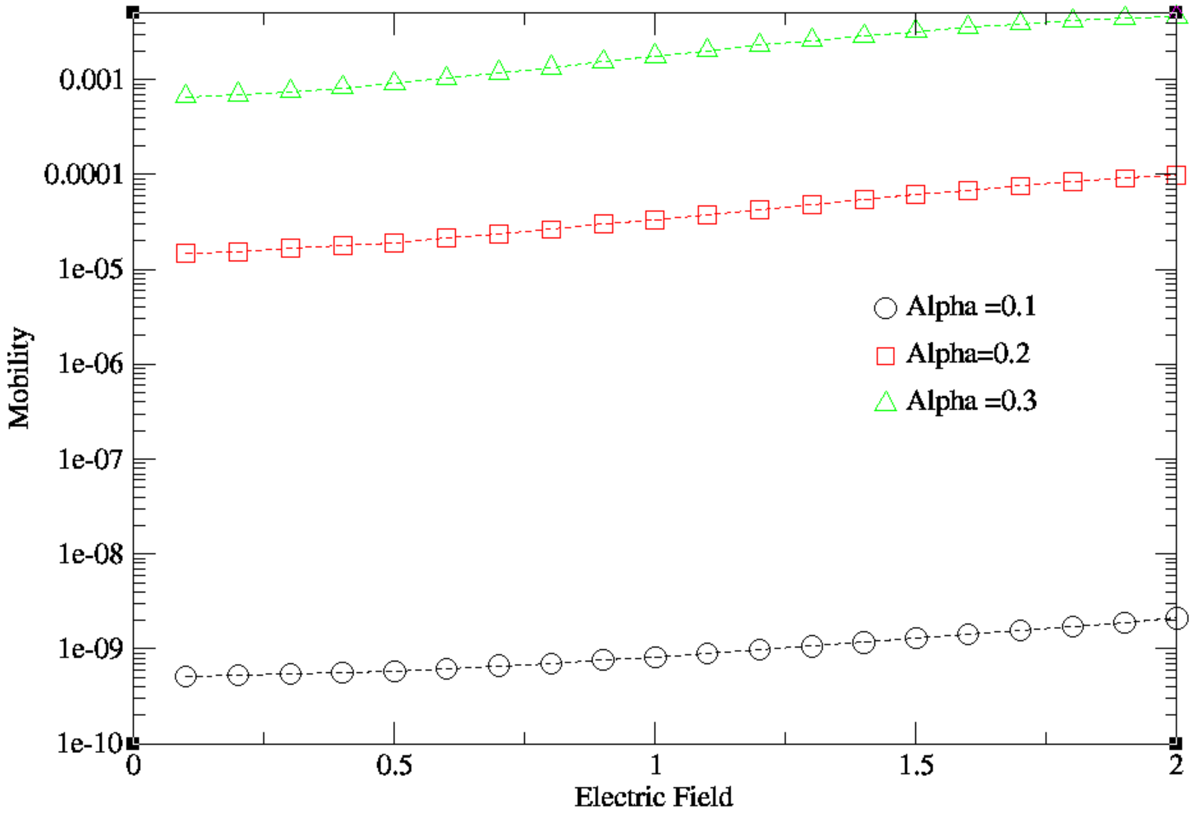

Figure 5.1: Mobility $\mu(F)$ versus electric field ($\sigma/e\alpha$) for localization length α (α for $\sigma/kT = 3$).

The Montecarlo simulation shown in Figure 5.1 shows the plot of mobility

$\mu(F)$ verses electric field ($\sigma/e\alpha$) for localization length α ($\sigma/kT = 3$) . It shows that the localization length α of the charge carriers in the localized states is the only spatial parameter responsible for the dependence of the hopping mobility μ on the applied electric field. As localization length increases, mobility of charge carriers increases and as the electric field increases, mobility of charge carriers also increases significantly. The localization length α, not the intersite distance $N^{-1/3}$ (presented in Equation 3.6 in the form of lattice constant "b"), is the decisive scale for the dependence of $\mu(F)$.

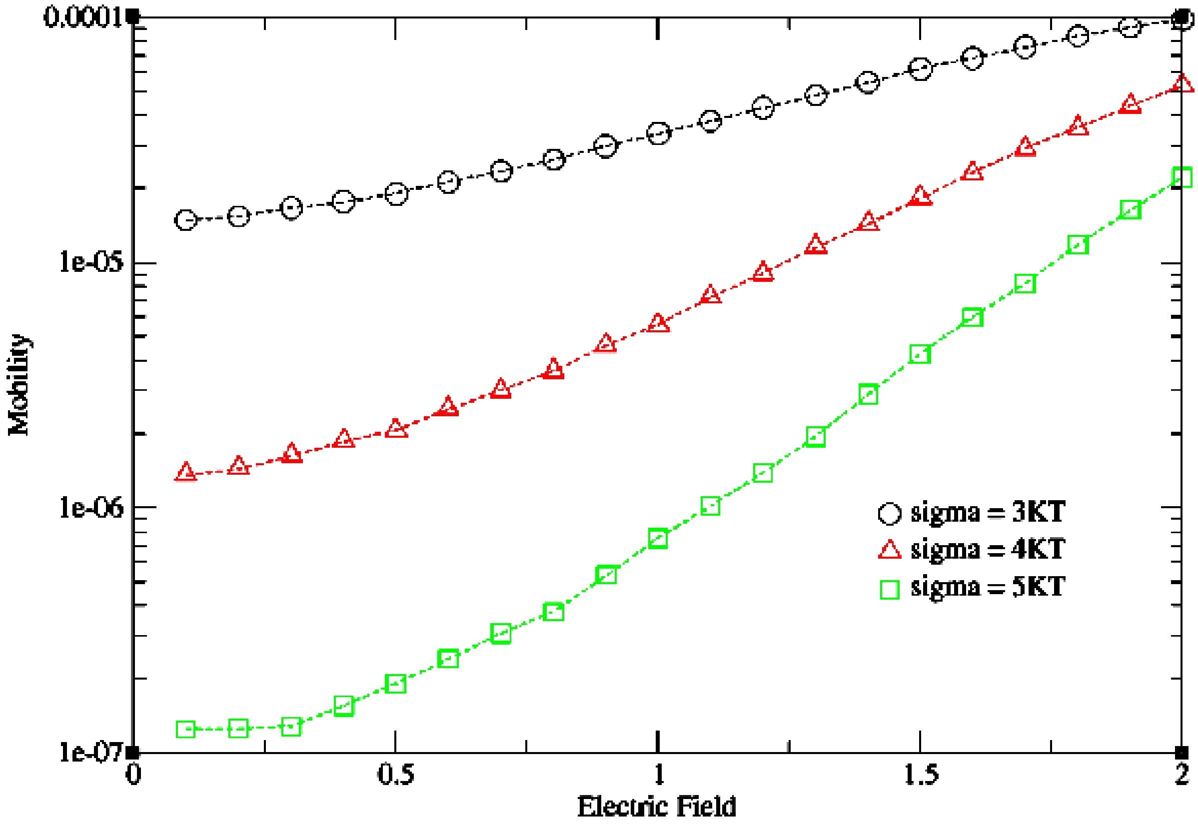

Figure 5.2: Mobility (μ/F) versus Electric field ($\sigma/e\alpha$) for different sigma ($\sigma/kT = 3$, $\sigma/kT = 4$ and $\sigma/kT = 5$) for localization length (α) 0.2.

Figure 5.2 shows the Montecarlo simulation plotted for $\mu(F)$ verses electric field F with the input parameters $\sigma/KT = 3$, $\sigma/KT = 4$ and $\sigma/KT = 5$. It shows that it resembles the Poole-Frenkle law which describes the escape of charge carriers from charge trap into transport band and mobility experience constant at low fields, mobility decreases for rising sigma (σ) but for far $\sigma = 5KT$, mobility increases for rising electric field and totally saturate at high fields. In addition, the simulation result indicates that the functional form of mobility as well as the parameter value B in Equation 3.4 are hardly influenced by structural disorder. While providing universal explanation for observed carrier mobility in structural disorder, $\ln \mu \propto \sqrt{E}$, low reproduced only narrow range.

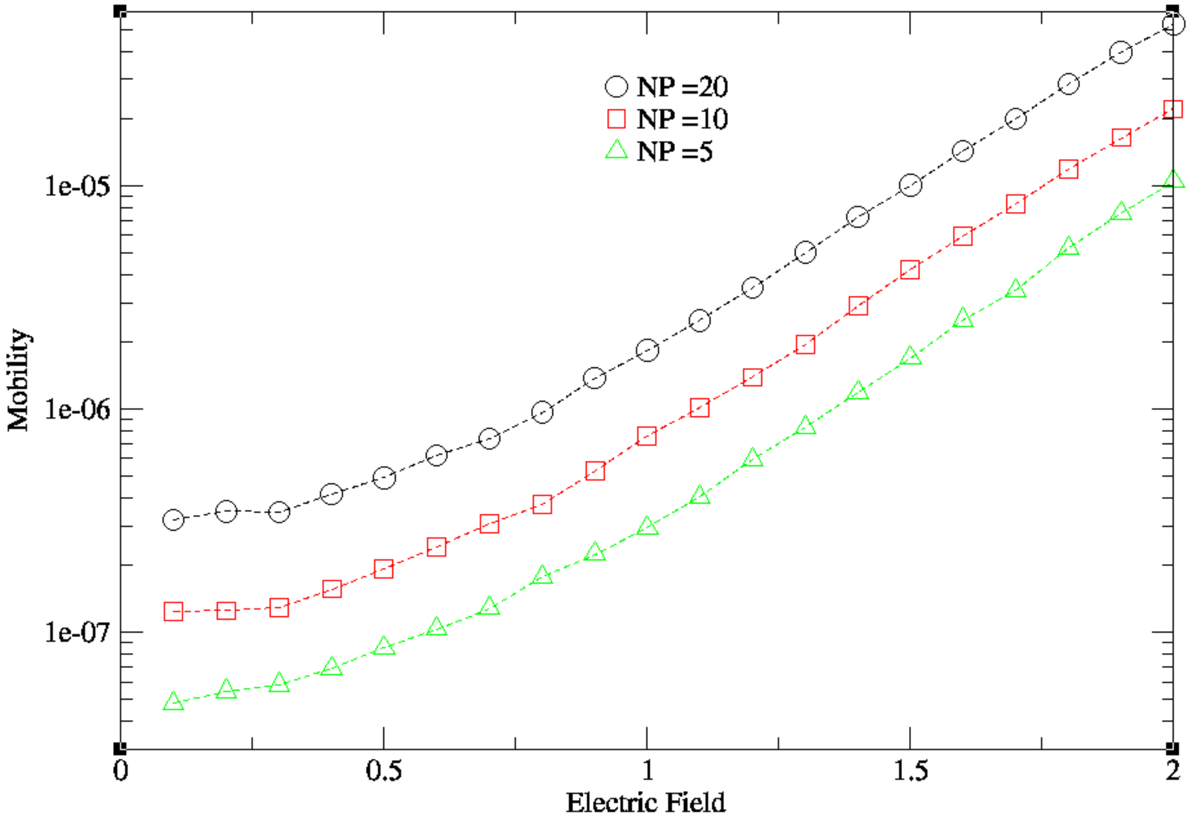

Figure 5.3: Mobility ($\mu(F)$) versus Electric field ($\sigma/e\alpha$) for different N_p (density of particle) and $N_p = 20(2 \times 10^{16} cm^{-3})$, $N_p = 10(10^{16} cm^{-3})$, $N_p = 5(5 \times 10^{15} cm^{-3})$, for $\sigma/kT = 5$, localization length (α) 0.2.

Figure 5.3 shows the Montecarlo simulation plotted for mobility $\mu(F)$ verses different densities, $N_P = 5$, $N_P = 10$, $N_P = 20$ and $\sigma = 5KT$. It shows that mobility is constant at low electric field. Mobility increases highly as the field rises and N_P (densities) increase, the mobility of charge carriers also increases.

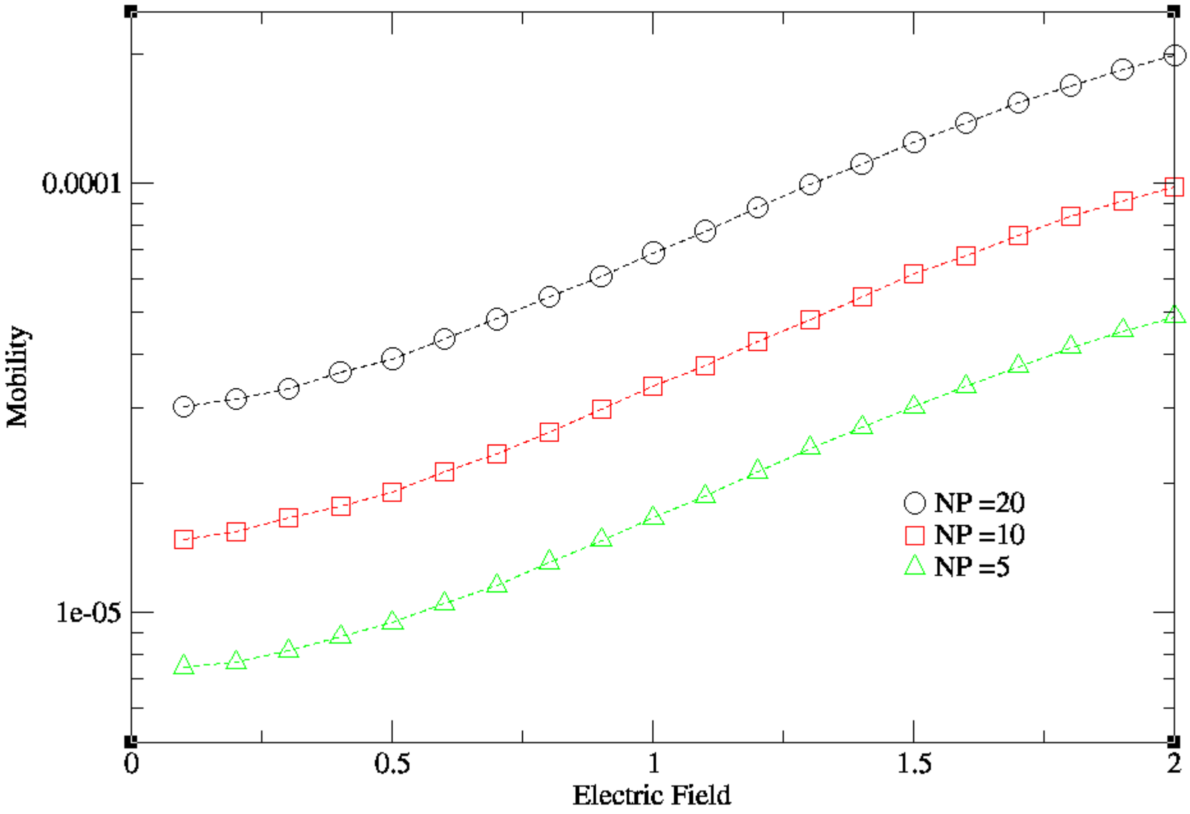

Figure 5.4: Mobility ($\mu(F)$) versus Electric field ($\sigma/e\alpha$) for different N_p (density of particle) and $N_p = 20(2 \times 10^{16} cm^{-3})$, $N_p = 10(10^{16} cm^{-3})$, $N_p = 5(5 \times 10^{15} cm^{-3})$, for $\sigma/kT = 3$, localization length (α) 0.2.

Figure 5.4 shows the Montecarlo simulation plotted for mobility $\mu(F)$ verses different densities N_p ($N_p = 5$,$N_p = 10$, $N_p = 20$) and for $\sigma/kT = 3$. It is similar to Figure 4.3 but in this case mobility increases highly as the value of sigma σ decreases. For both simulation plots in Figures 4.3 and 4.4, the electric field dependence of mobility for the two DOS width $\sigma/kT = 5$ and $\sigma/kT = 3$ charge densities, the electric field dependence of mobility at low charge densities can be fitted to the emperical equation derived by Bassler (Eq. (3.4)).

Chapter 6

Conclusion

In the previous chapter, the results of the Montecarlo simulation on charge carrier mobility variation with different localization length(α), sigma (σ/kT) for the applied electric field is described. This chapter presents the conclusions made based on the results obtained from the Montecarlo simulation.

The plot of the Montecarlo simulation in Figure 5.1 shows the dependence of charge carrier mobility $\mu(F)$ for different localization radii. It indicates that the localization length α of charge carriers in localization sites is the only spatial parameter responsible for dependence of hopping mobility μ on applied field in the system of random sites. It is clearly visible that α has large influence on the mobility. Large localization radii lead to much faster conduction than low value of α. This is expected since localization length (α) assists tunneling transitions between the site (the Miller-Abraham hopping rate Equation (1.5)1. Remarkably, this parameter α is not present in Equations 3.4 and 3.6, which is often treated as theoretical predictions for $\mu(F)$ and used in devices of simulations.

The plot of the Montecarlo simulation in Figure 5.2 indicates that, in low electric field regime, the charge carrier mobility remains constant. When the field increases, the mobility will increase as well, but the mobility will saturate when the field is beyond a certain threshold. The emperical Poole-Frenkel form, $\sigma \propto \exp(\gamma\sqrt{F})$, is only valid for the medium field regime.

The plots of the Montecarlo simulation in Figure 5.3 and 5.4 indicates that, the electric field dependence of charge carrier mobility for two DOS width (σ) charge densities or the electric field dependence at low charge densities can be fitted to the emperical equations derived by Bässler et al. based on Monte-Carlo simulations (Equation 3.4) . However, as the charge density (σ) goes up, the field dependence mobility is significantly reduced, and the dependence on σ is suppressed as well.

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DECLARATION

I, hereby, declare that this Master of Science project is my original work and it has not been presented for a degree for any other university and that all sources of materials used for the project have been dully acknowledge.

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