EFFECTS OF ELECTRIC FIELD ON A CHARGE CARRIER MOBILITY IN DISORDERED ORGANIC SEMICONDUCTORS FOR DIFFERENT LOCALIZATION LENGTH (MONTE CARLO SIMULATION)

A THESIS SUBMITTED TO

THE DEPARTMENT OF PHYSICS

IN PARTIAL FULFILLMENT FOR THE REQUIREMENT OF THE DEGREE OF Master of Science (PHYSICS)

By

Mebrhit Nguse Tewele

ADDIS ABABA UNIVERSITY

ADDIS ABABA, ETHIOPIA

SEPTEMBER 2020

ADDIS ABABA UNIVERSITY

EFFECTS OF ELECTRIC FIELD ON A CHARGE CARRIER MOBILITY IN DISORDERED ORGANIC SEMICONDUCTORS FOR DIFFERENT LOCALIZATION LENGTH (MONTE CARLO SIMULATION)

By

Mebrhit Nguse Tewele

Department of Physics

Addis Ababa University

Approved by the Examining Board:

Dr.Lemmi Demeyu Advisor	Signature
Dr.Kenate Numera Examiner	Signature
Dr.Yitagesu Elfagd Examiner	Signature
Dr. Deribe Hirpo Graduate program Chairman	Signature

Date: September 2020

ADDIS ABABA UNIVERSITY

Date: **September 2020**

Author: **Mebrhit Nguse Tewele**

Title: **Effects of electric field on a charge carrier mobility in disordered organic semiconductors for different localization length (Monte Carlo simulation)**

Department: **Department of Physics**

Degree: **M.Sc.** Convocation: **August** Year: **2020**

Permission is herewith granted to Addis Ababa University to circulate and to have copied for non-commercial purposes, at its discretion, the above title upon the request of individuals or institutions.

Signature of Author

Table of Contents

List of Figures

Acknowledgements

First of all, I would like to thank the almighty God for letting me accomplish this stage. I would like to thank my supervisor and advisor Dr. Lemi Demeyu for the opportunity to do thesis under his supervision while actually getting paid for it, and to his bravery in getting me started (and forcing me to finish!) on a topic which was partly new territory for me, but very exciting to me, for his guidance, encouragement, advice and assistance were indisputable to the completion of this work during this thesis. I am really indebted to him, without his help and patience, it is impossible to finish this great work, but also it assistance and advice is not only during this time, he advice and helps for the next of my life. So he is not only my advisor but also he helps and advise me as my father. My biggest thanks to the truly amazing Dr. Kenate Nmera who has spent an enormous amount of time to help me to install ubuntu and all softwore that I use in my thesis. I would like to thank for all my instructors of physics department for all support during my study. My strongest thank is addressed to all my Family members, specially to my daughter Meron Mebrahtom she is the heroine of my success. Because with out her push and support, this stage is unthinkable. I also thank all my intimate friends. Finally I would like to thank Addis Ababa Education Bureau for giving me this chance and also financial support.

Acronyms

VRH = variable range hopping

KMCS = kinetic Monte Carlo simulation

HOMO = higher occupied molecular orbital

LUMO = lower unoccupied molecular orbital

k = Boltzmann constant

eV = electron volt

E = electric field

$\widehat{\sigma}$ = Gaussian width (disorder material)

ODSs = organic disorder semiconductors

PFETs = polymeric field effect transistors

PLEDs = polymeric light emitting diods

MCM = Monte Carlo method

PV = photovoltaic

TFTs = thin film transistors

μ = mobility

GDM = Gaussian disorder model

Abstract

Organic semiconductors (OSCs) have attracted increasing interest since they have proven to be a potential use as active material in electronic devices such as organic light emitting diodes (OLEDs) and organic field effect transistors (OFETs). They are composed of molecules which are held together by Van-der Waals forces which are weak compared to covalent bonds and because of this OSCs are flexible and fabricated easily at low temperature. Van-derWaals bonding has an effect of forming narrow electronic bandwidths and weak intermolecular interactions which in turn lead to special and energetic disorder, and also localization of charge carriers. Thus, the charge carrier mobility in organic semiconductors is generally much smaller than that in covalently bonded crystalline inorganic semiconductors. Besides this one of the problems for the practical applications of organic semiconductor is lack of an understanding of charge carrier transport properties.

In this thesis, we investigate the charge carrier transport behavior of numerical code we developed using Kinetic Monte Carlo (KMC) simulation technique on the basis of Miller and Abrahams rate equation. Particularly we will show the mobility of charge carrier as function of electric field taking into consideration the effects of temperature, disorder parameter (known as Gaussian width), localization length and charge carrier density. In our simulation, the results will compare by variation of localization length, charge carrier density and Gaussian width.

CHAPTER 1
Introduction

Organic semiconductor attracts currently much attention in the scientific communty as materials are desired for applications in electronic devices such as organic field effect transistor, solar cells and light emitting diodes. Organic semiconductors (OSCs) are a class of carbon based materials that exhibit optical and electronic properties. They cover a large class of materials with broad varriety of properties. They can be fabricated in crystalline form, for instance pentacene and ruberene [1] and also in amorphous. The interest in organic disordered semiconductor (ODS) is caused by their optoelectronic featurs and by easy manufacturing, as compared to organic crystals.

In contrary to crystalline materials, ODS posses neither structural regularity nor spatially extended elctronic states. Instead electronic states in organic disordered semiconductors (ODSs) are spetially localized [2]. This happens because the overlap integrals for the weak van-der-walls interactions between neighboring stractural units (molecular) complexes in ODSs are much smaller than the energy scale of disorder, which prevents the formation of extended electronic states. Therefore charge transport in ODS is due to incoherent tunneling (hopping) of charge carriers between localized states that are randomly distributed in space.
Currently electronic properties of organic disordered semiconductors (ODSs) are focus on the intensive experimental and theoretical research. Due to thier potential applications in electronic devices such as light emitting diodes (OLEDs) [3], [4], field effect transistors (OFETs) [5] and organic solar cells (OSCs) [6] are intensively worked on. In our case the charge carrier transport parameter in ODS as function of temperature, charge carrier density, Gaussian disorder and electric field are investigated.

The most popular theoretical model to describe charge transport in ODS is Gaussian disorder model. According to this model the energies of charge carriers at localized sites are uncorrelated and distributed according to Gaussian distribution [7]. Hence the density of states (DOS) of disordered organic semiconductor is given by

$$g(\varepsilon) = \frac{N}{\sqrt{2\pi\sigma^2}} exp\left(\frac{-\varepsilon^2}{2\sigma^2}\right), \tag{1.1}$$

where σ is the characteristic energy scale of the disorder (which have a value $\sigma \sim 0.05 - 0.14eV$), N is concentration of localized states typically between N $\simeq 10^{20}cm^{-3}$ and N $\simeq 10^{21}cm^{-3}$, ε is the energy of a charge carrier when it is at a certain site.

Organic semiconductors are the key active component for the whole field of organic electronics. Organic semiconductor based devices have received much attention due to their good solution processability, low temperature deposition, low cost, and compatibility with large area printing technology.
Although the conventional amorphous silicon based semicoductors have achieved much progress with charge carrier mobility around $1.0cm^2V^{-1}s^{-1}$, the thin film deposition of conventional semiconductor usually needs high temperature process and dustless conditions which significantly increase the fabricating cost [8]. An understanding of the mechanisms that control the mobility of charge carrier is centeral to the operation of organic semiconductor devices. Charge carrier mobility in disordered localized states has been calculated mostly using Kinetic Monte Carlo (KMC) simulation technique [9].

Charge carrier conductivity (transport) is one of the key parameters that determine the performance of electronic devices. Transport in organic semiconductor refers to how charges move through a material with application of an electric field. It involves also the process of energy transfer from one site to another on the same chaine [10]. We focus how charge carriers in disordered organic semiconductor are transported. Organic semiconductors with a Gaussian density of states and with on site energies are uncorrelated. Charge transport in polymers and organic small molecule material occurs by thermally assisted tunneling between localized molecular states [11]. In this case we consider the transport in 3D disordered semiconductor to which electric field is applied only along and direction. Mobility

is one of the importance parameter that determine the charge carrier transport properties and the necessity of material for applications. Mobility of charge carrier is calculated as a function of applied electric field for different localization length, temperature, charge carrier density and disorder parameter using Kinetic Monte Carlo simulation technique.

1.1 Objective of the study

1.1.1 General objective

The goal of this thesis is to study charge transport and properties of charge carriers in ODSs using KMCS technique as function of electric field. The main transport parameter (mobility) depends on different parameter such as localization length, Gaussian width (disorder parameter), charge carrier density and temperature. The charge transport mechanisms in this material is by hopping from one site to another (between uncorrelated states).

1.1.2 Spesfic objective

The main goal of the thesis is to calculate mobility in hopping charge transport in the presence of applied electric field. Distinguish the difference between normalized and unnormalized slope of mobility from the graph. Express the relationship between mobility and electric field. To examine the factor affects of the on site energy on a hopping charge carrier transport when an electric field is applied along the x-axis. To identify the probability that a charge carrier hops from occupied site i to unoccupied site j in 3D model with maximum distnication site of 26. To simulate mobility of charge carrier in disorder organic semiconductor at different localization length, Gaussian width (disorder parameter), charge carrier density and temperature.

The rest of this thesis is organized as follows. Chapter two describes the overview of the transport of charge in disordered organic semiconductor, charge transport in organic semiconductor, valence and conduction band, hopping transport, transport of charge carrier in the presence of electrical field, charge carrier mobility, time of flight method and factor influencing of charge carrier mobility. Chapter three describes the model and method. The results will be discussed in chapter four. The summary and conclusion will be presented in chapter five.

CHAPTER 2

Over view of charge transport in disordered organic semiconductors

In this chapter we focus on the theoretical description of charge transport in a disordered organic semiconductors. Charge transport in conjugated polymer and molecular semiconductor is influenced by the molecular structure as well as the intermolecular interaction. Charge carrier mobility in conjugated polymer depends on intrachain and interchain interactions, mediated mainly by thermally activated hopping.

The characteristics of charge transport in organic semiconductor is one of the key attributes that impacts the performance of organic electronic devices in which they are utlized. Improving the performance of electronic device presupposes an understanding of charge carrier transport in organic semiconductors. Due to this reason it is important to know the transport behaviours of charge carrier in organic semiconductors. The fundamental understanding of charge transport mechanisms and the structural property relationships in organic semiconductors have been studied extensively in attempt to improved charge transfer rate [9].

2.1 Charge carrier transport in organic semiconductors

A material can conduct electric current only if there are free charge carriers in it. In metals the free charge carriers, electrons are available. In semiconductors, whether they are inorganic or organic there are no free charge carriers at low temperatures close to zero. At higher temperature some of electrons in the valence band move to conduction band leaving holes behind in the valence band.

Consquently, free charge carriers, both electrons and holes can be introduced in to inorganic semiconductors at high temperatures. This is not viable in the case of an organic semiconductor. Since its band gap is very large cmpared to thermal energy

at room temperature. However free charge carriers, either electron or hole, can be introduced in to both organic and inorganic semiconductors by doping chemically with impurity, illuminating with photons, and injecting from metal contacts. These free charge carriers move randomly in a diffusive manner when there is no external applied field. In the presence of external field, the free charge carriers experience unbalanced force and acquires a motion in a direction of the force, which is known as drift velocity (ν_d).

The drift speed is related to the applied electric field as $\nu_d = \mu E$, where μ is the mobility of the charge carrier in the material and E is the magnitued of the applied electric field. This means that the conductivity of a charge carrier in a material under the action of external bias depends on the charge carrier mobility in the material. Therefore, the mobility is a basic transport parameter, since it has direct relation with the conductivity. The studies that have been done so far have shown that the mobility depends on the disorder (or crystalinity) of a material, the charge carrier density, temperature, localization length and external applied electric field. In organic and disordered inorganic semiconductors there are defects or kinks that forms localized states.
This behaviour has influence on the mobility of charge carrier in the material besides its influence on the type of transport or conduction. It means that, charge transport in disordered organic semiconductors is goverend by hopping of charge carrier between localized states. For this resoan, mobility in organic semiconductor is found to be much smaller than that inorganic semiconductors.

Semiconductor is a material that has an electrical conductivity between a conductor and an insulator. The charge transport in disordered organic semiconductor takes place through a hopping of charge carrier between localized states on molecules or polymer segments.
To understand charge carrier transport in organic semiconductors, the temperature and electric field dependent of the hole mobility are the fundamental parameter [12]. In disorder organic semiconductors, transport of charge carriers are localized over spatially and energetically distributed. It is widely accepted that, the transport mechanism is hopping of charge carriers from one localized state to another with in a lattice of molecular site [13]. Many modern electronic devices such

as organic field effect transistor, organic light emitting diode and solar cell in today's are generally based up on non crystalline materials such as organic semiconductors [14], [15], [16] or amorphous silicon.

In a semiconductor, the valence band edge is the highest electron energy in which electrons are normally present at absolute zero temperature. At high temperature, the electrons are moving from valence band to conduction band [17]. **Valence and Conduction band** are the two different energy levels separated by band gap. Band gap is the energy difference between valence band and conduction band. Valence band is the electron band from which the electrons can jump out when the atom is excited, the electrons jump in to the condution band and it exist below the band gap. Conduction band is the energy level which is consists of free electrons and exists above the band gap, that is at higher energy state. If the electrons are in conduction band, these electrons have enough energy to move freely inside a material. This movement creates an electronic current. These electrons have greater mobility and responsible for electrical conductivity. At room

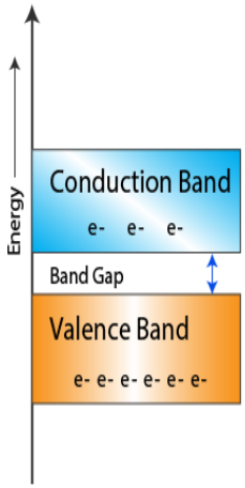

Figure 2.1: shows conduction and valence band of a semiconductor

temperature, the valence band is usually either partially or completely filled, but conduction band is generally empty or partially filled. Valence band is lower energy level, but conduction band is high energy level [18].

2.1.1 Hopping transport

The electronic wave functions are localized to molecular segments usually called sites, between which a charge carrier tunnel or hop so as to move through the system. In disordered organic semiconductors tunneling or hopping transitions of electrons between localized states in the band tails dominate the charge carrier transport. This transport regime is called hopping conduction, since an incoherent sequence of tunneling transitions of charge carriers resembles a series of their hops between randomly distributed sites. Each sites in this structure provide a specially localized charge carrier state with energy which is called site energy. We assume that the localized states for a number of charge carriers distributed in lattice sites with energies that are found from a density of states described by a Gaussian distribution function described by Eq. (1.1).

Considering that the absorption bands of amorphous organic semiconductors are typically found to exhibit a Gaussian shape, it is generally accepted that the density of state is appropriately described with a Gaussian distribution.
The modern description of hopping transport in a disordered system is simplified by employing the concepts of the effective transport energy. Charge transport depends on the ability of the charge carriers to pass from one molecule to another. Hopping between localized sites with a Gaussian energy distribution is a widely used model for describing charge carrier transport in disordered organic semiconductors. The hops from one site to another depends on the energy difference between the sites.

The hopping rates of charge carrier from an occupied site to an empty site is usually assumed to be described by the Miller-Abrhams expression [19].

$$\nu_{ij} = \nu_0 exp\left(\frac{-2|\overrightarrow{r}_{ij}|}{\alpha}\right)\gamma(\varepsilon_j - \varepsilon_i + eE.r_{ij}), \tag{2.1}$$

with

$$\gamma(\triangle\varepsilon) = \begin{cases} exp(\frac{-\triangle\varepsilon}{kT}), if\, \Delta\varepsilon{>}0 \\ 1, otherwise \end{cases} \tag{2.2}$$

where α is the localization length of charge carriers in the localized state which describes the decay strength of the localized wave functions; in disordered organic semiconductor which is estimated at the order of $10^{-8}cm$. E is the electric field, and ν_0 is a prefactor called escape frequency which has a value in the order of $10^{12}s^{-1}$, ε_i and ε_j are the on site energies of charge carrier at site i and j respectively,

$|\overrightarrow{r_{ij}}| = \overrightarrow{r_j} - \overrightarrow{r_i}$, $\overrightarrow{r_j}$ and $\overrightarrow{r_i}$ are the position of charge carrier at site j and i respectively, k is the Boltzmann constant and T is the absolute temperature. This equation consists of two exponentially decaying factors. The first one is the tunneling part of the rates which accounts for the distance between the sites that take part in the transition, and the second exponential function accounts for the energy difference between the sites.

The group of Bässler [7], [20], [21] simulated $\mu(E)$ on a cubic lattice and fitted results in the form of the parametrized equation.

$$\mu(E) = \mu_0 exp\Big\{ -\left(\frac{2\sigma}{3kT}\right)^2 \Big\} \times exp\Big\{ C\left[\left(\frac{\sigma}{kT}\right)^2 - B\right]\sqrt{E}. \Big\}, \tag{2.3}$$

where μ_0 is a field independent prefactor, E is electric field, σ is the standared deviation, k is the Boltzmann constant and T is absolute temperature.
Two parameters, C and B are involved in this fitting. The parameter C is assumed to depend on the lattice constant (distance between localization sites).
Equation (2.3) is one of the most frequently used equations in the context of organic semiconductors. A similar approach to determine $\mu(E)$ was used by Pasveer et al [22], who reduced the lattice Gaussian disorder model (GDM) of Bässler. Calculating numerically $\mu(E)$ in the framework of this reduced Gaussian disordered model (GDM) on a cubic lattice, Pasveer fitted results to the analytical formula.

$$\mu(T, n, E) \approx \mu(T, n)\Phi(T, E) \tag{2.4}$$

with $\Phi(T, E)$ in the form

$$\Phi(T, E) = exp\Big\{ 0.44\left[\left(\frac{\sigma}{kT}\right)^{3/2} - 2.2\right] \times \left[\sqrt{1 + 0.8\left(\frac{Eeb}{\sigma}\right)^2} - 1\right]\Big\}, \tag{2.5}$$

where b is the lattice constant. Charge transport properties are decisive in operating of devices, hence correct theoritical description of charge transport is a matter of major importance. Simple phenomenological models, first the Gaussian disorder model (GDM) by Bässler forms a basis of theoretical description and modeling of charge transport in disordered organic semiconductors. In the above two equations, Eqs. (2.3 and 2.5), a parameter called localization length was not involved which infact has influence on the hopping transport. In this work, we involve localization length and perform Kinetic Monte Carlo simulation are investigate charge transport in disordered organic semiconductors according to Miller-Abrahams rate equation as shown in Eq. (2.1).

The charge carrier density in organic disordered semiconductor depends on the energy gap between LUMO and HOMO. The charge carrier transport in disorder organic semiconductor is the aggregate of each charge carrier hopping between sites as shown in Fig. (2.2). The black circle on the site indicates that the charge

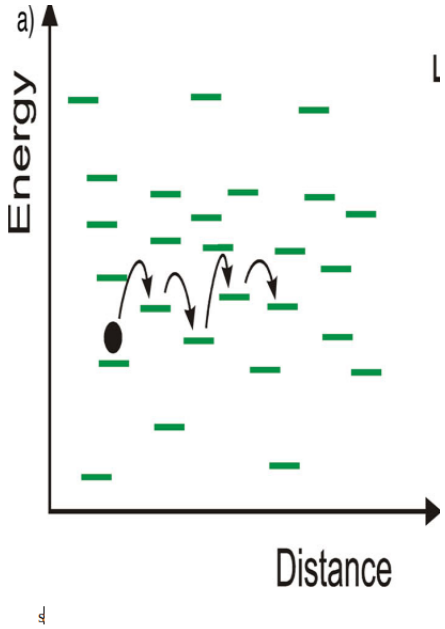

Figure 2.2: shows schematic drawings of the charge carrier hopping process in a disordered system

carrier particle that can hop from one site to another according to the energy difference between the sites, and the line shows the probability of disorder sites. Charge transport in disordered organic semiconductor is governed by variable range hopping (VRH) among a system of localized state. Variable range hopping is the general regime of hopping transport which is also valid at low temperature. In this work, we propose a VRH based charge transport model in three dimensional organic semiconductor system, which gives a field dependent conductivity (mobility) [23]. Variable range hopping is closely connected with the Millers and Abrahams hopping rates.

2.2 Transport of a charge carrier in the presence of electrical field

When an electric field is applied in an organic material, charge carriers will start to drift in the direction of the field. The analysis of transport of charge carriers in a material layer is made focusing on the drift of charge carriers in the presence of

local electrical field. Charge transport in disordered organic semiconductor refers to how charges move through a material with the application of an electric field. The electrical current density has two basic components, the conduction current and displacement current, the total electrical current density is given by

$$j_{tot} = j_{cond} + j_{disp} \tag{2.6}$$

The displacement current is associated with the time variation of electric field:

$$j_{disp} = \varepsilon \frac{dE}{dt}, \tag{2.7}$$

where ε is the parameter of dielectric material. Normally the displacement current is a transient effect associated with the charging of dielectric capacitance in the system. The conduction current density is related to the transport of charge carriers by the applications of a driving force. The current density at a cross section of the layer is a combination of the current carried by the different charge carriers in the system.

$$j = \sum_i j_i, \tag{2.8}$$

where j_i is the current carried by different charge carriers for i system. The total electrical current across the device is

$$I = Aj = A \sum_i j_i \tag{2.9}$$

, where A is the cross section area of the device, j_i is the current carried density for different i system. The average velocilty ν_i is determined by the product of the particle mechanical mobility B_i and the force F_i.

$$\nu_i = B_i F_i. \tag{2.10}$$

We consider the transport of charge carrier of concentration of number of particle per cm^3 and a charge number Z_i so that its electrical charge is:

$$Q = z_i q, \tag{2.11}$$

where q is elementary charge, Z_i charge number. The electrical force on a particle is

$$F_i = q z_i E. \tag{2.12}$$

For electronic carrier, the holes drift in the direction of the electrical field and the electrons against the field.

$$\nu_i = B_i q z_i E. \tag{2.13}$$

The carrier mobility is defined as the velocity per unit electrical field ($cm^2V^{-1}s^{-1}$).

$$\nu_i = \frac{z_i}{|z_i|}\mu_i E. \tag{2.14}$$

From the above equation charge carrier mobility is defined by

$$\mu_i = |z_i| q B_i. \tag{2.15}$$

Electronic carrier mobility in a semiconductor is strongly dependent on scattering process. Mobility is almost constant for low dopping concentrations and is bassically affected by phonon scattering. At higher doping concentrations, mobilty decreases due to the scattering by ionized impurities. Mobilty in organic semiconductor is found to depend on the value of the electric field and it is well described by an expression known as Pool-Frenkel law.

$$\mu(E) = \mu_0 exp(\gamma\sqrt{E}), \tag{2.16}$$

here μ_0 is constant, the mobility of electrons or holes at zero field, and γ is the parameter describing the field dependece. The carrier flux density J is defined as the number of carriers crossing a unit area per second.

$$J_i = c_i \nu_i, \tag{2.17}$$

where ν_i denotes average velocity and c_i is charge density. The flux can orginate from drift, diffusion, or other mechanism such as convection. The motion of the charge carrier due to the electrical field is normally denoted as drift transport. The flux denisity asscіated with drift transport is given by

$$J_i = \frac{z_i}{|z_i|} c_i \mu_i E. \tag{2.18}$$

The electrical current density j carrierd is defined by

$$j_i = z_i q J_i = q|z_i| c_i \upsilon_i E. \tag{2.19}$$

In a situation of transport by drift due to an electrical field, the electrical conductivity σ_i of one specific carrier is defined by the relationship

$$j_i = \sigma_i . E \tag{2.20}$$

From Eq. (2.21) the conductivity of charge carrier i has the expresssion of

$$\sigma_i = |z_i| q c_i \mu_i. \tag{2.21}$$

The total electrical conductivity is given by

$$\sigma = \sum_i \sigma_i = \sum_i |z_i| q c_i \mu_i. \tag{2.22}$$

Electric field plays an important role for the charge carrier transport in organic semiconductors, and hence influences the relaxation effect, however, most of the relaxation models didn't take into account the electric field effect up to date [24].

2.3 Charge carrier mobility

Charge carrier drift mobility is an important parameter in organic semiconductors. The hopping transport in disordered organic semiconductors results in rather low charge carrier mobilities that are electric field dependent and thermaly activated. Investigations of these dependence can offer a lot of information about the charge transport processes in these disordered materials. Low charge carrier mobility is one of the basic reasons that restrict the realization and utlization of instruments according to the organic semiconductors. Mobility is one of the important physical attributes of organic semiconductors and it has a critical effect on their performance in a variety of applications. The charge carriers are strongly localized on molecules or molecular segments. Mobility is a basic and fundamental for transport of charge carriers in a material or semiconductors.

Mobility tests how fast an electron able to move through a metal or semiconductor in the existance of electric field. Mobility means the movment of charge carriers. Electrical mobilty is the ability of charged particles (such as elctrons or holes) to move through a medium in response to an electric field that is applied on them. It can move in the absence and in the presence of an electric field. In the absence of an applied electric field, the carrier exhibits random motion and the carriers move quickly through the semiconductor and frequently change direction. When an electric field is applied, the random motion still occurs but in addition, there is on average a net motion along the electric field. The performance of any organic devices depends on the magnitude of mobility of the charge carriers. Charge carrier mobility in a transistor determines how fast the device can be turrned on or off [25].

This means that charge carrier mobility (μ) is a critical parameter that limits the efficiencies of organic electronic devices such as organic field effect transistors (OFETs) [26] and organic photovoltaic cells [27]. It is known that the disorder has strong impact on charge transport in organic semiconducting film. It is generally accepted that charge carrier transport in such materials occurs by hopping between localized states that are disordered in space and energy. Therefore charge carrier mobilities in these materials are, as a rule, very low and strongly temperature and field dependent. This fact has been consistently described by a formalism based on hopping in a Gaussian density of states (DOS) distribution [7], [22]. This model is applied to the analysis of both the electric field and the temperature dependence of mobility. In disorder organic semiconductor dvice, we considered that localized condtions are randomly dispensed in both energy and space coordinates, and they build an unconnected array of sites.

High mobility permits quick device operation that required low cost electronics on wide areas with achievement meeting market demands. For amorphous its value is $5 \times 10^{-1} - 10^{-3} cm^2/Vs$. For organic semiconductors to be competentive with amorphous silicon they must approach $1 cm^2/Vs$. Where $1 cm^2/Vs$ is also a borderline value between the transport band regime and the hopping regime. If the mobility is significantly lower than one it is in the hopping regime, if it is significantly higher than one it is the band regime [28].

2.4 Characterization of charge carrier mobility

The characteristics of charge transport in organic semiconductor is one of the key attributes that impacts the performance of organic electronic and optoelectronic devices in which they are utlized. Carrier mobility is the quantity that characterizes of charge transport. Without any external potential, transport is purely dispersed and is commonly expressed by diffusion equation.

$$< x^2 >= nDt, \tag{2.23}$$

where x^2 denotets the mean square displacement of the charge, D is the difussion coeficient, t is the time and n represents an integer number for three dimensional (3D) system. The charge carrier mobility μ is related to the diffusion coefficient via

the Einstein-Smoluchowski equation

$$\mu = \frac{eD}{kT}, \tag{2.24}$$

where k is the Boltzmann constant and T is the absolute temperature. Diffusion should be seen as a local displacement of the charge around an average position, while drift induces a displacement of the average position. Drift is the effect that dominates the migration of the charges across an organic layer in the devices [29].

2.5 The time of flight method

Time of flight is an essential to stabilize experimental techniques for mobility measurements in disordered organic devices like polymers and molecularly doped polymers where the low molecular weight organic materials are spread out in a binder polymers. It is broadly used for determination of charge carrier mobility in organic semiconductors. It is a basic to measure a charge transit time like the time requires for a sheet of charge carriers photo generated near to one of the electrodes by vibrated to be bright light and to drift across the sample to the other electrode under an applied electric field.

A short vibration of absorbed light produce holes or electrons close to transparent contact and one species is extracted whereas the other drifts to the opposite contact.

And then, the photo generated holes or electrons move across the material toward another electrode depending on the polarity of the applied bias and the equivalence electric field in the range of $10^4 - 10^6 V/cm$, the photogenerated holes or electrons move across the material toward the second electrode. Then, the current at that electrode can be recorded as a function of time. Finally, for ordered materials, a sharp signal will be obtained, while for disordered systems, a broadening of the signal will occur because of the distribution of transient times across the material. The mobility of holes or electrons is estimated via the following equation

$$\mu = \frac{\upsilon}{E} = \frac{d}{Et} = \frac{d^2}{Vt}, \tag{2.25}$$

where d is the distance between the electrodes, E is the electric field, t is the average transient time, and V is the applied voltage. Time of flight measurements clearly show the impact of structural defects present in the material on charge carrier mobility [29]. Charge mobilities in organic materials were first measured with the TOF technique by Kepler [30] and Leblanc [31].

2.6 Factors influencing charge carrier mobility

Charge transport needs that the charge carriers to be able to migrate from molecule to molecule and it is neither trapped nor scattered. Charge carrier mobility affects by several reason for instance; charge carrier density, electric field, temperature, disorder and localization length [29].

2.6.1 Electric field

The dependence of mobility on electric field is different in the case of single crystal and disordered material. The field dependence on single crystal is observed only in ultrapure crystals along the directions increase to the highest charge mobility. According to this, an increase in electric field is observed to reduce mobility. In the case of disordered materials, large mobility is observed at high fields. At low fields, the charges control to the follow of the best percolation pathways and to the structural defects; but high electric field impose a stronger directionality and prevent the charges from moving around the defects, thereby reducing mobility [32].

2.6.2 Temperature

The dependence of charge carrier mobility on temperature is different in the case of single crystal and in disordered material. In a single crystal, the electrons and holes mobilities are generally decrease with temperature according to a power law evolution μ/T^{-n}. In high disordered way, transport generally proceeds via hopping and is thermally activated.
High temperature is used to improve the transport of charges by providing the energy needed to overcome the barrier created by energetic disorder [33].

CHAPTER 3

Methodology

3.1 Monte Carlo simulation

In this chapter we discuss Monte Carlo simulation method used to calculate mobility on the hopping of charge carriers. We consider a three dimensional semiconducting polymer film that can be used as active material in electronic devices such like organic field effect transistors (OFETs). And we assume that there are free charge carriers in this material. When an external electric field is applied along the length of this material the charge carriers drift in this direction. The drift speed (or the drift mobility) of the charge carriers depend on the electric field, the morphology of the material, the temperature and the localization length.
In general mobility is not a linear function of these parameters and because of this it is not simple to analyze its relation with these parameters analytically. But, we can investigate the relation of transport parameter (mobility) with the parameters that have effect on it in disordered organic semiconductor numerically using computer simulation. One of these methods is Monte Carlo simulation.

Monte Carlo methods are a large class of computational algorithms that rely on random number generations, or random number sampling and it is a computerized numerical technigue. And also it is used in physics and mathematical problem and is most useful when it is difficult or impossible to use other approaches. It is a primary tool for extracting physical information corresponding to the charge transport process in disordered organic semicondutors under the premise of the Gaussian disordered model. In our case, its significance is for calculating charge carrier mobility in three dimensional system.
The Monte Carlo method is applied to solve different variety of problems. In statistical physics, it is used to investigate systems that obey Boltzmann statistics. The generation of a set of random numbers is essential to any Monte Carlo method,

irrespective of the applications. In MC simulation high number of samples are required to get a value that has good accuracy. This needs fast process which is usually achieved using an algorithmic approach for the generation of the numbers instead of a truly random number approach where it is impossible to predict the next number in the sequence.
An algorithmic approach to random number generation is given by

$$x_{i+1} = f(x_{i,parameter}). \tag{3.1}$$

The random numbers can be thought of as a sequence, where the next number in the sequence comes from applying a function taking some arbitrary parameters to the current number. This means that as long as the function f and the parameters are known, the next number in the sequence can be predicted and is in one sence not random at all. This is the reason why numbers generated by a computer in this way is often called Pseudo-random number. Fortunately, as long as the function f chosen in a clever enough way, for the vast majority of applications there is no difference between Pseudo-random numbers and random numbers that can not be predicted. A simple example of a pseudo-random number generator is the linear congruential random number generator. It is defined by the function

$$f(x, a, c, M) = (ax + c) mod M), \tag{3.2}$$

where a, c and M are the parameters. A good Pseudo-random number generator should from a Pseudo-random number that have a uniform distribution in the interval [0,1] which has a long period. Hopping transport of charge carriers can be described in different methods of MC simulation, such as Metropolis Monte Carlo and Kinetic Monte Carlo simulations. In our study we use KMC since it involves the time taken between sequence of equilibrium states of the system of charge carriers in organic semiconducting polymers. The purpose of Kinetic Monte Carlo is to reflect the time evolution of the system and to reproduce non equilibrium processes. It is a method used for solving kinetic Equations. In contrast to the equilibrium nature of the Metropolis algorithm, the Kinetic Monte Carlo method is well suited for studying time dependent pheneomena such as diffusion processes. KMC is used to identify how we can generate state when it moves from state i to state j. KMC method has a different scheme for the generation of the next state. The main idea behind KMC is to use transition rates that depends on the energy barrier between the states, with time increments formulated so that they relate

to the microscopic kinetics of the system. But, metropolis Monte Carlo simulation samples configurational space and generates configurational according to the desired statistical mechanics distribution without taking in to consideration the time taken between neighbouring states, and the method can not be used to study evolution of the system or kinetics. An alternative computional technique that can be used to study kinetics of slow processes is the Kinetic Monte Carlo method. In metropolis Monte Carlo method we decide whether to accept a move by considering the energy difference between the states [34] [35].

The Monte Carlo technique is relatively easy to carry out, in a particular way where the sites are situated regularly in three dimensional. The simplest approach is to place a single charge carrier (a hole in this case) at a time on a site or avoid double occupancy. This corresponds to a low charge carrier density, where Coulomb interaction among charge carriers is ignored. A charge carrier performs a random walk in the system of sites. The mobility is determined by performing MC simulation using a computer program based on FORTRAN 90 code. In the simulation, the destination site of every hopping charge carrier is chosen randomly, however it is measured by the hopping rate of likely destination site. The spending time on every site of charge carrier is also randomly chosen and it depends on the total rate of hopping of that site. For a single charge carrier the neighboring sites to which particle can hop is 26.

The Model

The sample of the material is modeled as a simple cubic lattice of $L_x \times L_y \times L_z$ sites, where L_x, L_y and L_z denotes the number of the lattice sites in the direction of x, y and z respectively. The lattice parameter is a which has a value about 1nm. Periodic boundary conditions are considered along all the three dimensions. Then N_p number of charge carriers are randomly distributed over the lattice sites. If the lattice parameter is 1nm the density of lattice sites is $10^{21}/cm^3$ whereas the density of the charge carriers is less than this (mostly) from $10^{15}/cm^3$ to $10^{18}/cm^3$. The appled electric field $\overrightarrow{E}$ in the system is directed along the x-axis. The on site energies of the charge carriers at all sites are randomly taken from a Gaussian distribution type density of states known width centered at zero energy. The energies are uncorrelated.

The electric potential energy of the charge carrier at each site due to the applied electric field is calculated and add to each of the on site energy at the corresponding sites. The transition rate of a charge carrier from an occupied site i to an empty site j which are separeted from each other by a distance r_{ij} is calculated using Miller-Abraham rate equation described by Eq. (2.1). Here the rectangular coordinates of all the sites are known in the code during the three dimensional sites formation. And the charge carriers are also identified with the number from 1 to N_p given to them when they are first introduced to the sites. It means that the coordinates of each charge carrier are known at every moment in the code, and the magnitude of the distance between any two destination and initial positions of a charge carrier that hops can be numerically calulated.

Our MC simulation procedures strat by forming the three dimension lattice of $L_x \times L_y \times L_z$ unoccupied sites. In the second step we calculate the on site disorder energies and electric potential energies for each site. In the third step we introduce N_p number of charge carriers to the system by randomly placing them on the unoccupied sites formed in the first procedure. In the fourth step, the exact three dimensinal charge carrier distribution influenced by the energies introduced above are realized. Initially, the charge carriers are distributed randomly throughout the total volume of the sample. Then, the steady state distribution is obtained via the MC steps. That means, we pick the first particle and check if its neighbouring sites are empty or occupied. If there is no empty sites the particle will remain at its position (or its hopping rate is recorded as zero) and we go to the second particle. But, there is neighbouring unoccupied site we calculate the total energy difference of the particle between the neighbouring empty sites and initial site. Then we solve for the transition rate, and repeat the same for all particles.
From these rates we find the normalized transition probabilities for each possible hopping rate. Based on the weight of the probability we move a charge carrier around; the probability that a charge carrier hops from an occupied site i to an empty site j is

$$p_{ij} = \frac{\nu_{ij}}{\sum_{i=1}^{N_p} \sum_{j=1}^{26} \nu_{ij}}, \tag{3.3}$$

here the summation is done over all possible hops of all the particles and the total probabilities is normalized to 1. This shows that the probabilities are a sequence of length intervals between 0 and 1. To decide for a particalar hop we generate a

random number from a uniform distribution also in the interval between 0 and 1, which points at a particular interval and consequently at a particular destination site to which the charge carrier then hops.
We have restricted the possible destination sites j to the 26 nearest neighbour sites of each charge carrier. If more number of possible destinations are involved, since the majority of the hopping events occur to the nearest neighbouring sites, the effect of this restriction is negligible. As it is also computationally very expensive have avoided involving more number of possible destinations. The mean dwelling time t_{av} at site i is given by

$$t_{av} = \frac{1}{\sum_{i=1}^{N_p} \sum_{j=1}^{26} \nu_{ij}}, \tag{3.4}$$

where the minimum and maximum limits of approach zero and infinity, respectively. The probability distribution function per unit time is given by

$$p(t) = \frac{1}{t_{av}} e^{\frac{-t^{'}}{t_{av}}} \tag{3.5}$$

When we draw the random number r on the interval (0,1),

$$\int_0^t p(t)dt^{'} = r \tag{3.6}$$

$$\int_0^t \frac{1}{t_{av}} e^{\frac{-t^{'}}{t_{av}}} dt^{'} = r \tag{3.7}$$

$$\frac{1}{t_{av}} \left[t_{av} e^{\frac{-t^{'}}{t_{av}}} \right]_0^t = -r, \tag{3.8}$$

$e^{\frac{-t}{t_{av}}} - 1 = -r$, $e^{\frac{t}{t_{av}}} = 1 - r$. The exact dwelling time is approcimated from the relation $t = -t_{av} ln(1 - r)$, where r is a random number taken from a uniform distribution between 0 and 1.

We let the system pass through 5.5×10^5 MCTS to ensure that the system has reached a steady state distribution. One MCTS is the step in which the hopping of one particle is performed. It should be noted that different generations of the on-site energies from the Gaussian disorder model (GDM) results in small but not able differences in results. The results are therefore averaged over 15 different generations of energy distributions. The final step of our simulation procedure involves recording of the displacement of the charge carriers along the length in the direction of $\overrightarrow{E}$ together with the time taken for this displacement to take place. The recording is performed in the next 49.5×10^5 MCTS. The displacement of the charge carriers in the direction of the electric field divided by the time taken gives

the velocity, and the mobility of the charge carriers is obtained from the ratio of the velocity and the applied electric field.

$$\mu = v/E = \Delta x/tE. \tag{3.9}$$

Finally, simulation data are collected as a function of $\overrightarrow{E}$, for different charge carrier densities, temperature (T), disorder parameter (σ) and localization length (α).

CHAPTER 4
Results and discussion

The simulation have been performed on a sample consisting of $140 \times 140 \times 140$ sites with periodic boundary conditions in the x, y and z directions, while the electric field is applied only in x-direction, for different loclization length, charge carrier density and disordered parameter. If we use the Gaussian shape energy spectrum the simulations have been implemented for N_p particles. Our results are plotted for various number of charge carriers (N_p), localization length (α) and Gaussian width ($\widehat{\sigma} = \sigma/kT$). Each graph will be interpreted by considering the value of mobility.

4.1 Mobility as a function of electric field for different values of $\widehat{\sigma}$

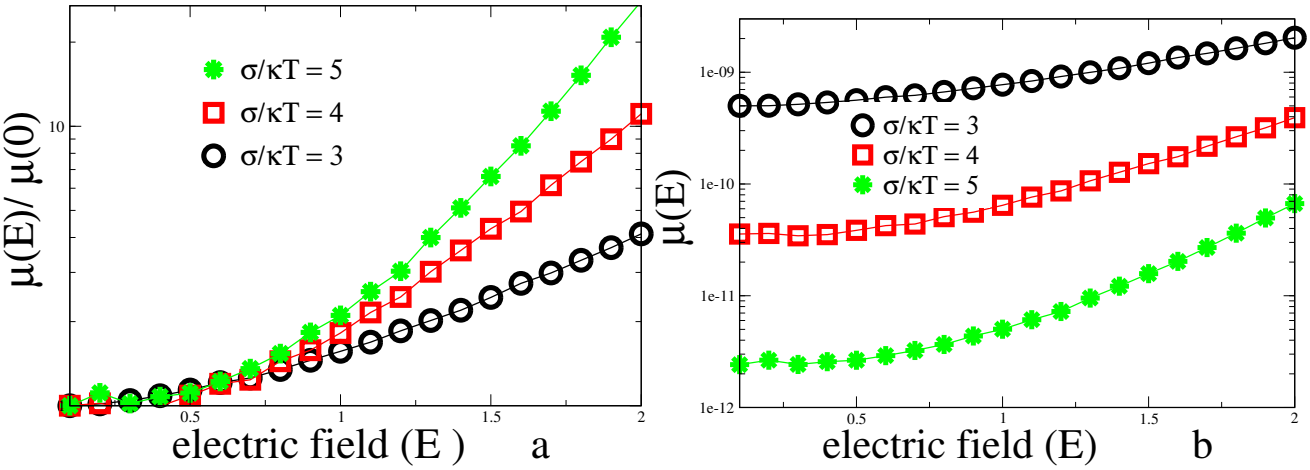

Figure 4.1: The plots in a and b show mobility versus electric field for various Gaussian width $(\widehat{\sigma})$, where $\widehat{\sigma} = \sigma/kT$. Fig. 4.1 (a) contains plots of mobility $(\mu(E)/\mu(0))$ versus electric field in unit of $(\frac{\sigma}{ea})$. It is normalized condition, which means the result gets by taking the ratio of mobility at different values of electric field to the mobility at minimum value.
Fig. 4.1 (b) are plots of mobility in a unit of μ_0 versus electric field. In both Figures, $\widehat{\sigma}$ is varies which is 3, 4 and 5, but the charge carrier density and localization length are constant ($N_p = 10$, α = 0.1).

We observe that mobility increases with increasing electric field. In both Figures the plotes become more steep when the disorder parameter increases. Fig. (4.1a) shows mobility ($\mu(E)/\mu(0)$) in logarithmic scale versus electric field in a unit (σ/ea) for various Gaussian width ($\widehat{\sigma}$). At $\widehat{\sigma} = 3$, the maximum and minimum value of mobility is 4 and 1, respectively, the plot is described by black circle. This slope presents slightly ramp. At $\widehat{\sigma} = 4$, the maximum and minimum value of mobility is 11 and 1, respectively, the plot is described by red square. At $\widehat{\sigma} = 5$, the maximum and minimum value of mobility is 27 and 1, respectively, the plot is described by green star.

Fig.(4.1b) also shows mobility on a logarithmic scale in the unit of μ_0 versus electric field in a uint of ($\frac{\sigma}{ea}$) for different $\widehat{\sigma}$. In this Figure we observe that mobility decreases with increasing Gaussian disorder, but mobility increases with increasing electric field. At $\widehat{\sigma}$ = 3, the maximum and minimum values of mobility is 2×10^{-9} and 5×10^{-10}, respectively, the plot is described by black circle. At $\widehat{\sigma}$ = 4, the maximum and minimum values of mobility is 3×10^{-10} and 3.9×10^{-11}, respectively, the plot is described by red square. At $\widehat{\sigma}$ = 5, the maximum and minimum values of mobility is 6.6×10^{-11} and 2.4×10^{-12}, respectiely, the plot is described by the green star. Generally we observe that, the slope of mobility increases with increasing of $\widehat{\sigma}$ for normalization condition as shown in Fig. (4.1 a), but mobility decrease the with increasing of $\widehat{\sigma}$ for unnormalized condition as shown in Fig. (4.1 b). It has to be noted that mobility decreases when $\widehat{\sigma}$ increases. In other way, the slopes of mobility in normalized condition start at the same point and they move together for some spaces then they rise up steadily; after the value of elctric field 1 they begin to move scatteringly. The slope that is discribed by star ($\widehat{\sigma}$ = 5) is the highest of the slopes that discribed by square ($\widehat{\sigma}$ = 4) and by circle ($\widehat{\sigma}$ = 3) as shown in Fig. (4.1a). But the slopes of mobility in unnormalized condition starts at different points and they rise slightly upward. The slope of mobility at high disorder parameter ($\widehat{\sigma}$ = 5) is lowest of the others as shown in Fig. (4.1b)

4.2 Mobility as a function of electric field for different $\widehat{\sigma}$ and localization length

We observe that mobility increases with increasing electric field and localization length. The input parameters are constant except localization length and $\widehat{\sigma}$. When

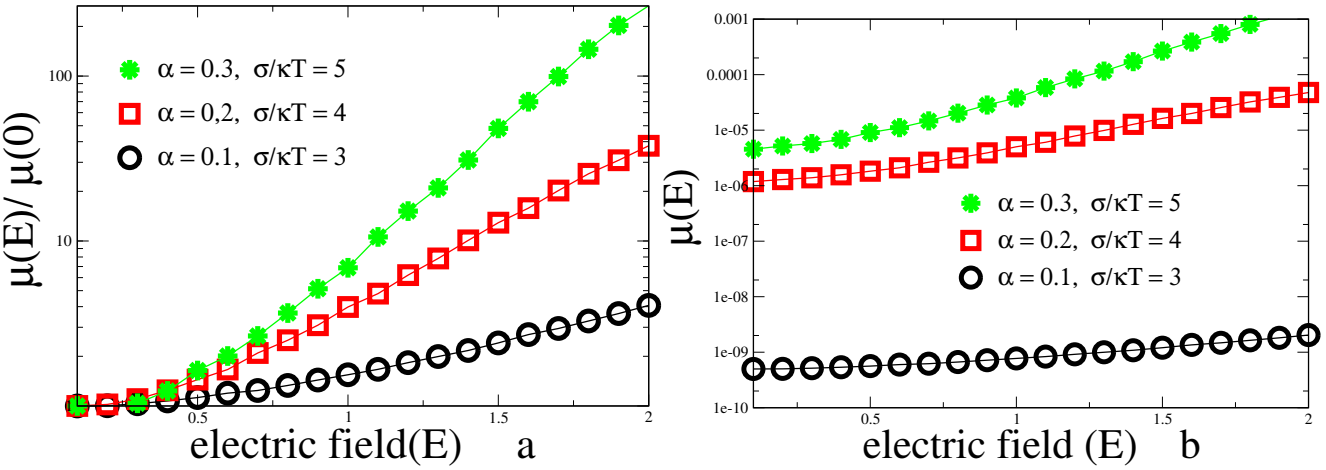

Figure 4.2: (a) The graphs of mobility ($\mu(E)/\mu(0)$) in logarithmic scale versus electric field in unit ($\frac{\sigma}{ea}$) for different disorder parameter ($\widehat{\sigma}$) and localization length (α). The result gets by taking ratio of mobility at different values of electric field to the mobility at minimum value.
(b) The graphs of mobility in a unit of μ_0 in logarithmic scale versus electric field in a unit of ($\frac{\sigma}{ea}$) in linear scale. In both cases ($\widehat{\sigma}$) is 3, 4 and 5, where $\widehat{\sigma} = \sigma/kT$ and localization length is 0.1, 0.2 and 0.3, but charge carrier density is constant which is 10.

both localization length and Gaussian disorder are vary at the same time, mobility become more increase. Fig. (4.2a) shows mobility in a unit of $\mu(E)$ in logarithmic scale versus electric field in a unit of ($\frac{\sigma}{ea}$) for different values of $\widehat{\sigma}$ and localization length. The maximum and minimum value of mobility is 266 and 1, respectively. The relative value of mobility with respect to that at minimum value increases very fast as a function of electric field at increasing both $\widehat{\sigma}$ and localization length at the same time. At $\widehat{\sigma}$ = 3 and α = 0.1nm, the maximum and minimum value of mobility is 4 and 1, respectively, the plot is described by black circle. At $\widehat{\sigma}$ = 4 and α = 0.2nm, the maximum and minimum values of mobility is 37.77 and 1, respectively, the plot is described by red square. At $\widehat{\sigma}$ = 5 and α = 0.3nm, the maximum and minimum values of mobility is 266.72 and 1, respectively, the plot is described by green square. When we compare the value of mobility in Fig. (4.1a) with that in Fig. (4.2a), the value of mobility in Fig. (4.1a) is smaller than the value of mobility in Fig. (4.2a). Because localization length in the first figure is constant which is 0.1nm, but for the second figure the localization length is different. The position of the curve is at the bottom for the minimum values of localization length and Gaussian width. The curve is more slopping up ward at maximum localization length and Gaussian width than that for minimum values of localization length and Gaussian width. This justifies that the hopping charge carrier is more dependents on

the value of localization length. Mobility increases with increasing localization length and electric field. The curve is more slopping up ward at maximum value of localization length and Gaussian width.

Fig. (4.2b) shows mobility in logarithmic scale in a unit μ_0 versus electric field in a unit ($\frac{\sigma}{ea}$) in linear scale for different Gaussian width and localization length, and the result gets without taking the ratio (the factor of $\widehat{\sigma}$). The input parameter in this figure is the same with taht of Fig. (4.2a). But the maximum and minimum value of mobility in this case is 1.5^{-3} and 5^{-10}, respectively, because mobility in this case is described in unnormalized condition. At $\widehat{\sigma}$ = 3 and α = 0.1nm, the maximium and minimum value of mobility is 2×10^{-9} and 4.99×10^{-10}, respectively, the plot is described by black circle. At $\widehat{\sigma}$ = 4 and α = 0.2nm, the maximum and minimum value of mobility is 4.7×10^{-5} and 1.1×10^{-6}, respectively, the plot is described by red square. At $\widehat{\sigma}$ = 5 and α = 0.3nm, the maximum and minimum value of mobility is 1.5×10^{-3} and 4.5×10^{-6}, respectively, the plot is described by green star. The plot becomes at the top for maximum value of localization length and becomes at the bottom for minimum value of localization length. The value of mobility in Fig. (4.1b) is much smaller than mobility in Fig. (4.2a). The plot is more slopping up ward at maximum value of localization length and Gaussian width. The value of mobility is more increases with increasing both localization length and Gaussian width at the same time. The position of the curve is at the bottom for the minimum value of localization length and Gaussian width. And the plot is at the top for the maximum value of localization length and Gaussian width. Therefor mobility increases with increasing localization length and decreases with increasing Gaussian disorder. Genarally we observe that, maximum mobility gets at maximum value of localization length and Gaussian width.

4.3 Mobility as a function of electric field for different localization length for constant $\widehat{\sigma}$

We observed that mobility increases with increasing electric field and localization length. The input parameters are constant except localization length which is considered to be 0.1, 0.2 and 0.3. In this case the main factor that affects of charge carrier mobility is localiation length, because the other input materials are constant. Fig. (4.3a) shows mobility ($\mu(E)/\mu(0)$) in logarithmic scale versus electric

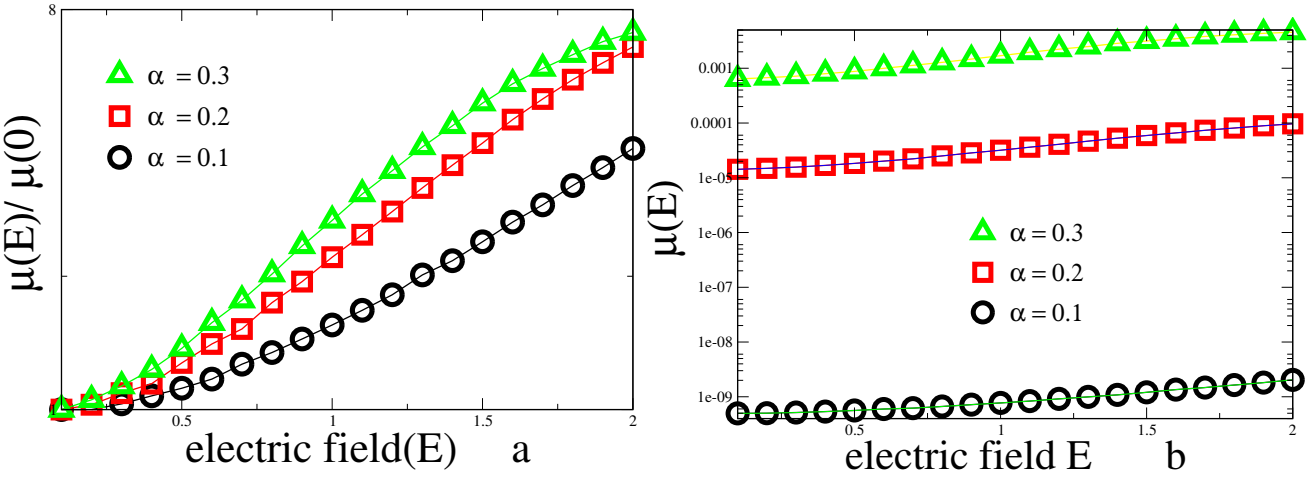

Figure 4.3: (a) The graph of mobility $(\mu(E)/\mu(0))$ in logarithmic scale versus electric field in a unit $(\frac{\sigma}{ea})$ in linear scale for various localization length. The result gets by taking the ratio of mobility at different value of electric field to mobility at minimum value.
(b) The graph of mobility $\mu(E)$ in logarithmic scale versus electric field in linear scale for various localization length, where $\mu(E)$ is with the unit of μ_0. In both Figures localization length varies which is 0.1 , 0.2 and 0.3, but the charge carrier density and Gaussian width are constant $(N_p = 10$, $\widehat{\sigma}$ = 3), where $\widehat{\sigma} = \sigma/kT$ and k is Boltzmann constant.

field for different localization length. For increasing localization length the mobility is found to increase. From calculation we get the maximum and minimum value of mobility is 7 and 1, respectively. At α = 0.1nm, the maximum and mnimum value of mobility is 3.88 and 1 respectively, the plot is described by black circle. At α = 0.2nm, the maximum and minimum value of mobility is 6.66 and 1, respectively, the plot is described by red square. At α = 0.3nm, the maximum and minimum value of mobility is 7 and 1, respectively, the slpoe becomes stastical graph which is described by green triangle up. The maximum value of mobility is at maximum value of localization length and the minimum mobility is for minimum value of localization length.

Fig. (4.3b) also shows mobility in a unit of μ_0 versus electric field in a uint of $\frac{\sigma}{ea}$ for different value of localization length (0.1, 0.2, 0.3). In this case the maximum and minimum value of mobility is 4.5×10^{-3} and 5×10^{-10}, respectively. For increasing localization length the curve of mobility is slopping upward.
At α = 0.1, the maximum and minimum value of mobility is 2×10^{-9} and 4.4×10^{-10}, respectively, the slope is slightly horizontal which is described by black circle. At

α = 0.2nm, the maximum and minimum value of localization length is 9×10^{-5} and 1.4×10^{-5}, respectively, the plot is described by red square. At α = 0.3nm the maximum and minimum value of mobility is 4.5×10^{-3} and 6.4×10^{-4}, rspectively, the plot is described by the green triangle up. The slope in this case is more scattered than the slopes in Fig. (4.3a).

For increasing localization length mobility also increase. The slope of these graphs is flat at minimum value of localization length and its slope becomes steeply upward for the maximum localization length. When we compare the value of mobility in Fig. (4.1b and 4.3b), mobility in Fig. (4.3b) is greater than in Fig. (4.1b). The main cause for this result is in Fig. (4.1b) we varies Gaussian width whereas in Fig. (4.3b) we varies localization length. Therefore for normalization condition, large value of mobility gets with variation of Gaussian width (at large Gaussian width). For unnormalized condition, maximum mobility gets at maximum value of localization length. Generally, the charge carriers are hops from on site to another site depends on the amount of energy; which means the charge carriers can hop in to minimum amount of energy and the mobility becomes increases.

4.4 Mobility as a function of electric field for different localization length and $\widehat{\sigma}$

The graph shows mobility $(\mu(E)/\mu(0))$ versus electric field in units of $(\frac{\sigma}{ea})$. We observe that mobility increases with increasing electric field. Fig. (4.4a) shows mobility versus electric field for differnt Gaussian width and constant localization length. The value of Gaussin width in this case is 3, 4 and 5 and localization length is 0.1. In this graph we obsreve that the slope of mobility is increasing with increasing Gaussian width. At $\widehat{\sigma}$ = 3, the maximum and minimum value of mobility is 4 and 1, respectively, the plot is described by the black circle. At $\widehat{\sigma}$ = 4, the maximum and minium value of mobility is 10.89 and 1, respectively, the plot is described by red square. At $\widehat{\sigma}$ = 5, the maximum and minium value of mobility is 20.97 and 1, respectively, the plot is described by green triangle up. The graph is steeply slopping upward at high Gaussian width.

Fig. (4.4b) shows mobility versus electric field for differnt localization length and constant Gaussian width. Localization length is 0.1, 0.2 and 0.3 and Gaussian

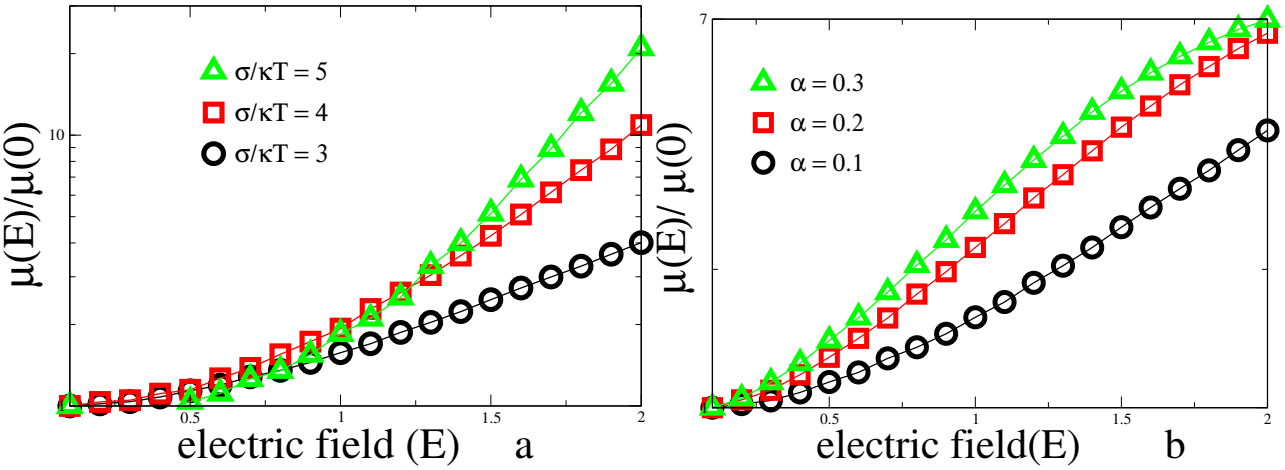

Figure 4.4: (a) The graph of mobility $(\mu(E)/\mu(0))$ in logarithmic scale versus electric field in a unit $(\frac{\sigma}{ea})$ for various Gaussian width $(\widehat{\sigma})$, which is 3, 4 and 5, where $\widehat{\sigma} = \sigma/kT$, k is the Boltzmann constant, but loclization length is constant which is 0.1nm.
(b) The graph of mobility $(\mu(E)/\mu(0))$ in logarithmic scale versus electric field in a unit $(\frac{\sigma}{ea})$ for various localization length, which is 0.1, 0.2 and 0.3 and Gaussian width is 3. Charge carrier density in both graphs is constant, which is 50.

disorder is 3. The slope of the mobility in this case also increases with increasing localization length. At α = 0.1nm, the maximum and minium value of mobility is 4 and 1, respectively, which is similar with Fig. (4.4a) and the plot is described by black circle. At α = 0.2nm, the maximum and minium value of mobility is 6.52 and 1, respectively, the plot is described by red square. At α = 0.3nm, the maximum and minium value of mobility is 7 and 1, respectively, its slope is stastical curve described by the green triangle up. The maximum value of mobility is obtained at maximum localization length which is 7. The graph is steeply slopping upward for increasing localization length. Generally from Figs. (4.4a and 4.4b) we observe that mobility in both cases become increase but its value is not the same. On these graph we understands mobility increases with increasing localization length, electric field and Gaussian width. In both case the calculation is normalized, which means the result gets by taking the ratio of mobility at different values of electric field to the mobility at minimum value. when we compare the value of mobility on these Figures with the above Figs. (4.1a, 4.2a and 4.3a), the value of mobility in Figs. (4.4a and 4.4b) is smaller than in Figs. (4.1a, 4.2a and 4.3a) because charge carrier density is different. Therefor in small charge carrier density the value of mobility becomes large.

4.5 Mobility as a function of electric field with different Gaussian width and charge carrier density

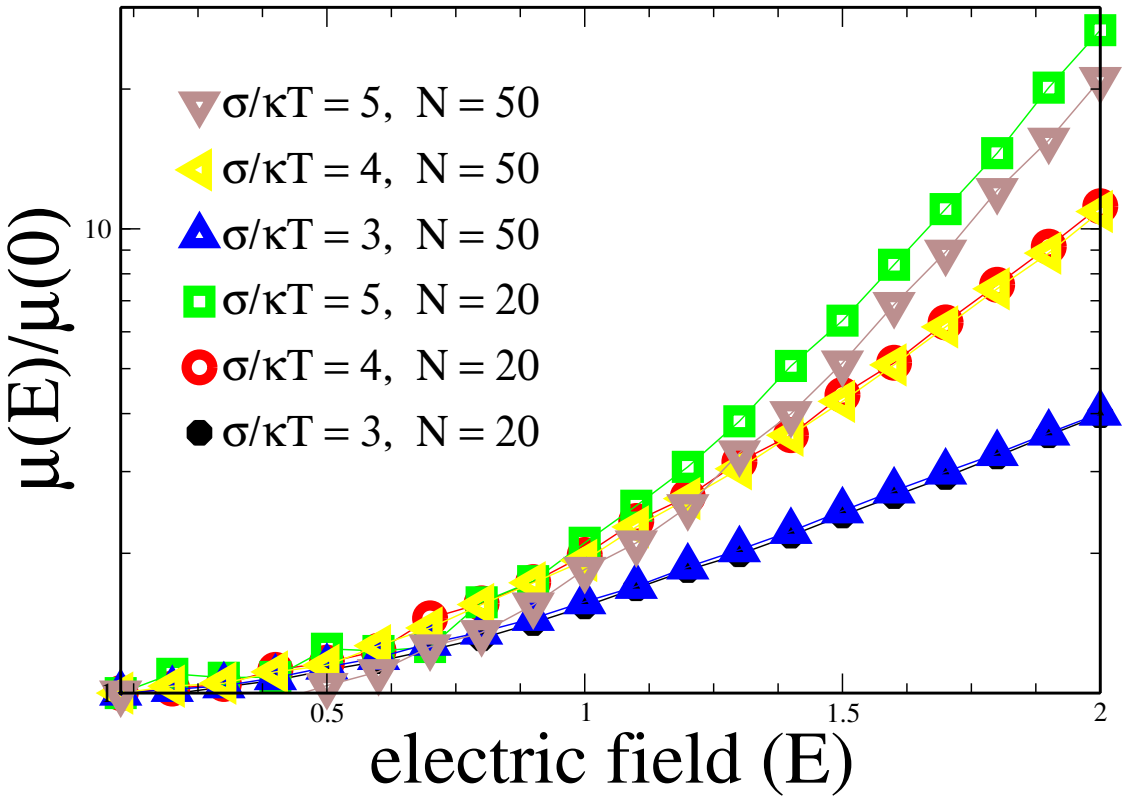

Figure 4.5: The graph of mobility $(\mu(E)/\mu(0))$ versus electric field in a unit $(\frac{\sigma}{ea})$ for different Gaussian width $(\widehat{\sigma})$ and the charge carrier density for the black star, red circle and green square is 20 and the charge carrier density for blue triangle up, yellow triangle left and brown triangle down is 50. The value of Gaussian width is ($\widehat{\sigma}$ = 3, 4 and 5), where $\widehat{\sigma} = \sigma/kT$ and localization length is constant which is 0.1nm.

Fig. (4.5) shows mobility versus electric field for different Gaussian width and the charge carrier density is 20 and 50. From this graph we observe that the slope of the mobility is steeply upward with increasing Gaussian width and electric field. At $\widehat{\sigma}$ = 3, the maximum and minimum value of mobility is 4 and 1, respectively, the plot is described by the black star. At $\widehat{\sigma}$ = 4, the maximum and minimum value of mobility is 11.18 and 1, respectively, the plot is described by red circle. At $\widehat{\sigma}$ = 5, the maximum and minimum value of mobility is 26.78 and 1, respectively, the plot is described by the green square. All these result gets from a charge carrier density of 20. At a charge carrier density $(N_p = 50)$, the value of mobility is described

as follow. At $\widehat{\sigma}$ = 3, the maximum and minimum value of mobility is 4 and 1, respectively, the plot is described by the blue triangle up. At $\widehat{\sigma}$ = 4, the maximum and minimum value of mobility is 10.8 and 1, respectively, the plot is described by yellow triangle left. At $\widehat{\sigma}$ = 5, the maximum and minimum value of mobility is 20.97 and 1, respectively, the plot is described by brown triangle down.

Therefore the main factor that affects for the value of mobility is charge carrier density. Because localization length and Gaussian width is the same, but charge carrier density is different. At charge carrier density of 20 and 50, the value of mobility is different. Then mobility becomes maximum at minimum value of charge carrier density, and minimum at maximum value of charge carrier density. Or in other word the maximum mobility obtained from the minimum value of charge carrier density. The slope of mobility is more increases at small number of charge carrier as shown in Figs. (4.5). But, at $\alpha = 0.1$ and $\widehat{\sigma} = 3$ respectively, the slope of mobility is approximatly the same in both case. Generally the result of mobility is obtained by taking the ratio of mobility at different value of electric field to mobility at minimum value.

4.6 Mobility as a function of electric field with different localization length

Fig. (4.6) shows mobility in logarithmic scale versus electric field in a unit ($\frac{\sigma}{ea}$). The main factor that affects for the slopes of mobility in this case is disorder parameter. We observed that mobility increase with increasing disorder parameter and localization length. We consider the slopes of mobility is in normalized condition, that is the result gets by taking the ratio of mobility at different value of electric field to mobility at minimum value. The slopes of mobility at different disorder parameter become varies. The slope described that by the green circle shows the slope of mobility at different localization length (α = 0.1, 0.2 and 0.3) but at constant disorder parameter which is ($\widehat{\sigma}$ = 3). At α = 0.1, $\widehat{\sigma}$ = 3, the maximum and minimum value of mobility is 4 and 1, respectively, the plot is described by green circle. At α = 0.2, $\widehat{\sigma}$ = 3, the maximum and minimum value of mobility is 6.6 and 1, respectively, the plot is described by green circle. At α = 0.3, $\widehat{\sigma}$ = 3, the maximum and minimum value of mobility is 7 and 1, respectively, the plot is described by green circle. All the slopes are sitting at the bottom of the boundary condition.

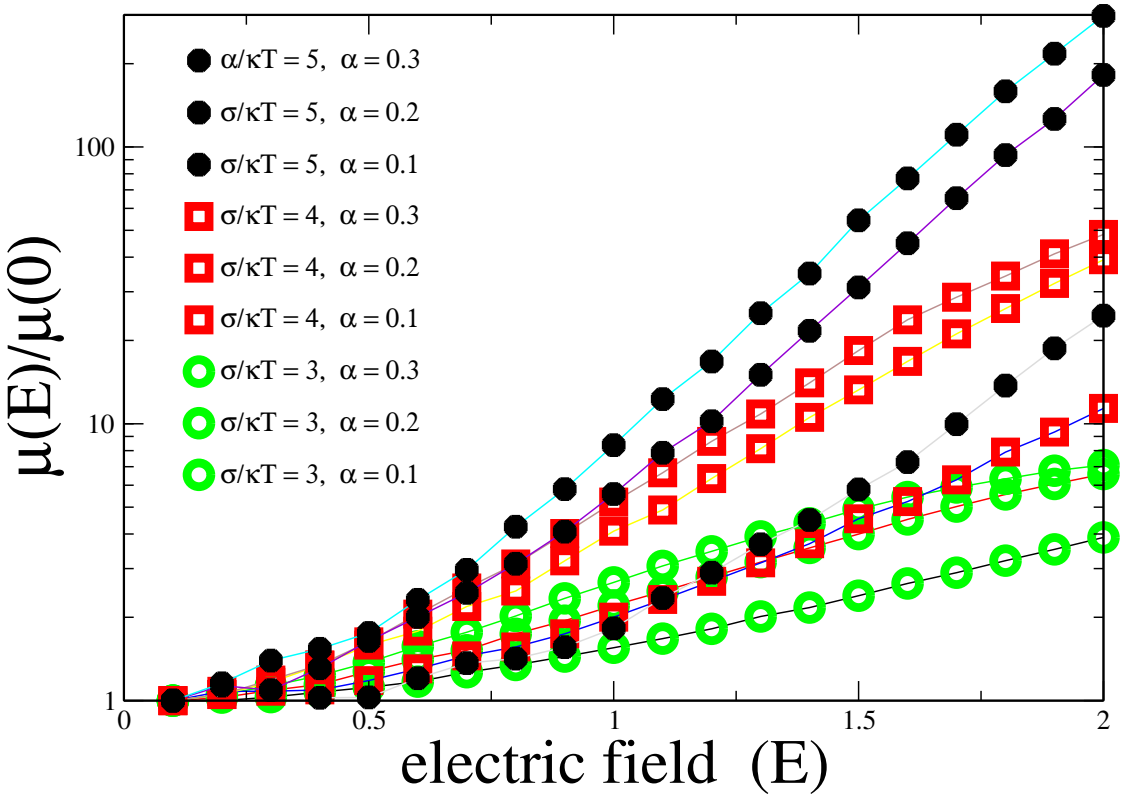

Figure 4.6: The graph of mobility $(\mu(E)/\mu(0))$ versus electric field (E). The Gaussian width for the green circle is $\widehat{\sigma}$ = 3, for the red square $\widehat{\sigma}$ = 4 and for the black star $\widehat{\sigma}$ = 5, where $\widehat{\sigma} = \sigma/kT$ and E is electric field in a unit of $(\frac{\sigma}{ea})$. But, localization length varies in the same value wich is α = 0.1, 0.2 and 0.3 and charge carrier density is constant which is 10. The result gets by taking the ratio of mobility at different value of electric field to the minimum value.

The slope described that by the red square shows the slope of mobility at different localization length (α = 0.1, 0.2 and 0.3) but at constant disorder parameter which is ($\widehat{\sigma}$ = 4). At α = 0.1, $\widehat{\sigma}$ = 4, the maximum and minimum value of mobility is 11.36 and 1, respectively, the plot is described by red square. At α = 0.2, $\widehat{\sigma}$ = 4, the maximum and minimum value of mobility is 39.13 and 1, respectively, the plot is described by red square. At α = 0.3, $\widehat{\sigma}$ = 4, the maximum and minimum value of mobility is 48.33 and 1, respectively, the plot is described by red square. The slopes of mobility in this case sitting at the middle of the boundary condition as shown in Fig. (4.6).

The slope described that by the black star shows the slope of mobility at different localization length (α = 0.1, 0.2 and 0.3) but at constant disorder parameter which is ($\widehat{\sigma}$ = 5). At α = 0.1, $\widehat{\sigma}$ = 5, the maximum and minimum value of mobility is 24.6 and 1, respectively, the plot is described by black star. At α = 0.2, $\widehat{\sigma}$ = 5, the maximum and minimum value of mobility is 182 and 1, respectively, the plot is described by black star. At α = 0.3, $\widehat{\sigma}$ = 5, the maximum and minimum value of mobility is 297.5 and 1, respectively, the plot is described by black star. The slopes in this case sitting at the top of boundary condition as shown in Fig. (4.6). When we compare the slopes of mobility in this graph, the plot becomes more slopping upward at maximum value of Gaussian width. Generally we observed that the slopes of mobility are starts at the same point and they move together for some spaces, and they begin to move scatteringly after the value of electric field 1. At higher Gaussian width ($\widehat{\sigma}$ = 5), the slope is rise sharply. The slope that is discribed by the black ($\widehat{\sigma}$ = 5) is the highest of the other slopes as shown in Figs. (4.6).

4.7 Mobility as a function of electric field with different $\widehat{\sigma}$ and localization length

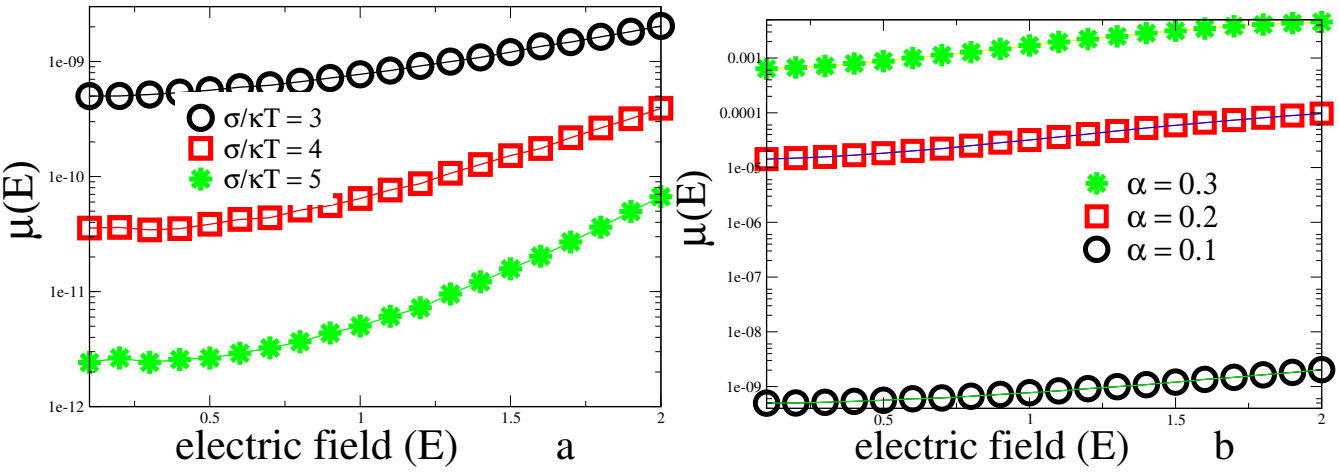

Figure 4.7: (a) The graphs of mobility ($(\mu(E))$) versus electric field for different Gaussian width ($\widehat{\sigma} = 3, 4, 5$), where $\widehat{\sigma} = \sigma/kT$ and localization length $(\alpha = 0.1)$. (b) The graphs of mobility ($\mu(E)$) versus electric field for different localization length ($\alpha = 0.1, 0.2, 0.3$) and $\widehat{\sigma} = 3$. Where $\mu(E)$ is mobility as function of E in a unit of μ_0. The charge carrier density in both a and b is constant which is $(N_p = 10)$.

We observe that mobility is increase with increasing electric field. The hopping

charge transport in both figures is in unnormalized condition. In this case the value of mobility is increases with increasing localization length. Fig. (4.7a) shows mobility versus electric field with various Gaussian width $(\widehat{\sigma})$, its value is 3, 4 and 5. Localization length is constant which is 0.1nm and charge carrier density is constant which is 10. This graph can interprate depends on the value of Gaussian width. When Gaussian width is 3, the maximum and minimum value of mobility is 2×10^{-9} and 5×10^{-10}, respectively, the plot is described by the black circle. At $\widehat{\sigma}$ = 4, the maximum and minimum value of mobility is 3×10^{-10} and 3.9×10^{-11}, respectively, the plot is described by red square. At $\widehat{\sigma}$ = 5, the maximum and minimum value of mobility is 6.6×10^{-11} and 2.4×10^{-12}, respectivly the plot is described by the green star. The slope that is discribed by green star is lowest from the other. From this we observes in unnormalized condition the slope of mobility is lowest at high Gaussian width.

Fig. (4.7b) shows mobility versus electric field for α = 0.1nm, 0.2nm and 0.3nm and $\widehat{\sigma}$ = 3. At α = 0.1nm, the maximum and minimum value of mobility is 2×10^{-9} and 4.9×10^{-10}, respectively, the plot is described by the black circle. At α = 0.2nm, the maximum and minimum value of mobility is 9×10^{-5} and 1×10^{-5}, respectively, the plot is described by the red square. At (α) = 0.3nm, the maximum and minimum value of mobility is 4.5×10^{-3} and 6×10^{-4}, respectively, the slope is described by green star. Generally in unnormalized condition the slope of mobility is highest for variation of localization length (at maximum localization length) as shown in Fig. (4.7b), but when we vary Gaussian width, maximum mobility obtains from minimum value of Gaussian width as shown in Fig. (4.7a).

CHAPTER 5

Summary and conclusions

We have performed simulations of hopping charge transport in disordered organic semiconductors. The transport model is based on hopping events between localized states with uncorrelated (random) on site energies. In this work we have Kinetic Monte Carlo simulation techniques widely used for the characterization of charge transport in disordered organic semiconductors. We observed that, mobility varies with variation of localization length, charge carrier density and Gaussian width. The maximum value of Gaussian width is considered to be 5 and the minimum value is 3. The slopes of mobility in the case of normalized condition are closely to each other. But, in unnormalized condition they are scatered.

And we observed that the slopes of mobility in normalized condition are arranged from minimum to maximum value of localization length whereas the slopes of mobility in unnormalized condition arranged from maximum to minimum according to the variation of Gaussian width. The slope of mobility starts at the same point in the case of normalyzed condition but in the case of unnormalyzed condition their starting point is different. The slope of mobility is steeply upward at high electric field. When localization length and electric field are increasing, mobility also increase. For normalized condition charge of mobility is fast (steeps) when the localization length and Gaussian width are large. For unnormalized condition mobility decrease with increasing Gaussian width. The highest value of mobility obtained at large value of electric field and localization length. Therefore we can generalize that localization length and electric field have significant effect on the mobility of charge carriers.

Bibliography

[1] O. Ostroverkhova, Chem. Rev. **116**, 13279 (2016).

[2] E. A. Silinsh, phys. stat. sol. (a) **3**, 817 (1970).

[3] C. W. Tang and S.A.Van Slyke, Appl. Phys. Lett. **51**, 913 (1987).

[4] J .H. Burroughes, D. D. C.Bradley, A. R. Brown, R. N.Marks, K. Mackay, R. H. Friend, P. L. Burns and A. B. Holmes, (Nature) **59**, 347 (1990).

[5] A. R. Brown, C. P. Jarrett, D. M. de Leeuw, and M. Matters, Synth. Met. **37** 88 (1997).

[6] A. Y. Kryukov, A. C. Saidov, and A. V. Vannikov, Thin Solid Films **84**, 209 (1992).

[7] H. Bässler, phys. stat. sol. B **175**, 15 (1993).

[8] V.R. Nikitenko, N.A. Sannikova and M.N. Strikhanov, Physics Procedia **72**, 431437 (2015).

[9] Kaiser, Waldemar, Albes, Tim, Gagliardi, and Alessio, Physical Chemistry Chemical Physics **20**, 8908 (2018).

[10] McCulloch, Iain and Heeney, Martin and Bailey,C.Bailey, Clare and Genevicius, Kristijonas and Shkunov, Maxim and Sparrowe, David and Tierney, Steve and Wagner, Robert and Zhang, Weimin and others, Nature materials, **pp.328** (2006).

[11] M. Bouhassoune and V. Meansfoort, SLM and P.A. Bobbert and R. Coehoorn, Organic Electronics **10**, 437- 445 (2009).

[12] N. Karl, Synthetic Metals **133**, 657 (2003).

[13] L.u. Nianduan and Li, Ling and Banerjee, Writam and Sun, Pengxiao and Gao, Nan and Liu, Ming, Journal of Applied Physics **118**, 045701 (2015).

[14] J. H. Burroughes, D. D. C. Bradley, A. R. Brown, R. N. Marks, K. Mackay, R. H. Friend, P. L. Burns, and A. B. Holmes, Nature **347**, 539 (1990).

[15] C. D. Dimitrakopoulos, S. Purushotaman, J. Kymissis, A. Callegari, and J. M. Shaw, Science **283**, 822 (1999).

[16] C. J. Brabec, N. S. Sariciftci, and J. C. Hummelen, Adv. Funct. Mater. **11**, 15 (2001)

[17] Fishchuk, II and A.K. Kadashchuk, and Genoe, Jan and Ullah, Mujeeb and H. Sitter, Singh, Th B and Sariciftci, NS and H. Bässler, Physical Review B **81**, 4 (2010).

[18] X.u. Yong, Schoonen, A.A. Martin, American Mineralogist **85**, 3-4 (2000).

[19] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).

[20] A. Köhler and H. Bässler, Electronic Processes in Organic Semiconductors (Wiley-VCH, Weinheim, 2015).

[21] P. M. Borsenberger, L. Pautmeier, and H. Bässler, J., Chem. Phys. **94**, 5447 (1991).

[22] W. F. Pasveer, J. Cottaar, C. Tanase, R. Coehoorn, P. A. Bobbert, P. W. M. Blom, D. M. de Leeuw, and M. A. J. Michels, Phys. Rev. Lett. **94**, 206601 (2005).

[23] L.Ling and S.V. Winckel, Steven and J.Genoe and P. Heremans, Applied physics letters **95**, 15 (2009).

[24] Bisquert Juan, Nanostructured energy devices: foundations of carrier transport **pp. 1-2**, 2017, CRC Press http://www.crcpress.com.

[25] C. D. Dimitrakopoulos, S. Purushotaman, J. Kymissis, A. Callegari, and J. M. Shaw, Science **283**, 822 (1999).

[26] C. J. Brabec, N. S. Sariciftci, and J. C. Hummelen, Adv. Funct. Mater. **11**, 15 (2001).

[27] R. Richert, L. Pautmeier, and H. Bässler, Phys. Rev. Lett. **63**, 547 (1989).

[28] R.J. Kline and M.D. McGehee, Macromolecular Science Part C: Polymer Reviews **46**, 2745 (2006).

[29] Coropceanu, Veaceslav and Cornil, Jérôme and da Silva Filho, Demetrio A and Olivier, Yoann and Silbey, Robert and Brédas, Jean-Luc, Chemical reviews **107**, 926-952, (2007).

[30] R.Kepler, G. Phys. Rev. **119**, 1226 (1960).

[31] O. H. J. Leblanc, Chem. Phys. **33**, 626 (1960).

[32] W. Warta, N. Karl, Phys. Rev. B **32**, 1172 (1985).

[33] N. Karl, K. Kraft, H. Marktanner, J. Munch, M. Schatz, F. Stehle, R. Uhde, H. M. J. Vacsci., Technol. A **17** 2318 (1999).

[34] H.Swendsen, Robert and J. S. Wang, Physical review letters **57**, 21 (1986).

[35] A. Levi and M. Kotrla, J. Cond. Matt. **9**, 299 (1997).

DECLARATION

I, here by, declare that this Master of Science thesis is my original work and it has not been presented for a degree in any other university and that all source of materials used for the thesis have been duly acknowledged.

Name of Candidate: Mebrhit Nguse Tewele

Signature: _____

E-mail: _____

Place and time of submission:
Addis Ababa University
Department of physics
Date: September 2020

Advisor
This thesis has been submitted for examination with my approval as a University advisor.

Name Dr. Lemi Demeyu

Signature: _____

E-mail _____