TRANSPORT PROPERTIES OF CHARGE CARRIERS IN ORGANIC POLYMER FILMS USED IN FIELD EFFECT TRANSISTOR

By

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Signature of Author

This Work is Dedicated

to

My mother, the greatest in the world.

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Acronyms and Abbreviations Used

OFETs - Organic Field Effect Transistors.

OPVs - Organic Photovolatics.

OLEDs - Organic Light Emmiting Diodes.

NNH - Nearest neighbor hopping.

LUMO - Lowest Unoccupied Molecular Orbital.

HOMO - Highest Occupied Molecular Orbital.

VRH - Variable range hopping.

GDM - Gaussian disordered model.

DOS - Density of state.

MC - Monte Carlo.

MD - Moleculare Dynamics.

MCS - Monte Carlo Simulation.

KMC - Kinetic Montecarlo.

PES - Potential energy surface.

2D - Two Dimensional.

3D - Three Dimensional.

SM - Simulation Methode.

TFTs - Thin film Transistors

Abstract

Application of a gate bias to an organic field-effect transistor leads to accumulation of the charge carriers in an organic semiconductor within a thin region near an interface of the gate dielectric. An important question raised by this study is whether the charge transport in the region can be affected by thickness layer of semiconductor, the morphology of active material and the gate bias are considered as the factor for varying charge carrier mobility for this particular study.

In order to answer this question, we have performed Montecarlo simulation of charge transport in organic field-effect transistor structure with a varying thickness of the organic layer, the gate bias, and the morphology of active material taking into account Coulomb interactions. We explain the charge carrier mobility as a function of field strength for disorder parameter $\hat{\sigma} = 4$ and $\hat{\sigma} = 3$ to draw a conclusion for strong disorder charge carrier mobility is good enough than weak disorder, For gate bias since the number of particles on metallic contact depend on the gate bias therefore when we increase the gate bias charge carrier mobility increases and for different organic layer thickness specifically up to the third layer the charge carrier mobility increase which leads us to a conclusion that charge transport in organic semiconductor layer should be considered three dimensional.

CHAPTER 1
INTRODUCTION

Organic semiconductors or plastic electronics have been widely studied since the 1970s following the discovery of conducting property of poly-acetylene by Alan Macdiarmid, Alan Heeger, and Hideki Shirakawa [1]. Their work resulted in Nobel prize in chemistry in 2000 for the discovery and development of conducting polymers. Since then the research on organic electronic devices based on inorganic semiconductors such as hydrogenated amorphous silicon for certain application.

It has become interesting due to its semiconducting properties for applications as active materials to existing and emerging technology such as organic photovoltaics (OPVs), organic light emitting diodes (OLEDs), and organic field effect transistors (OFETs) [2][3].

They are promising compared to conventional electronic devises based on inorganic semiconductors[4] because of their low cost fabrication, realization of large area display, environmentally friendly, and flexibility. Moreover organic materials can conduct both holes and electrons (or ambipolar) or conduct either holes or electrons where the electrons mobility is lower than that of hole mobility. Although a number of problems associated with organic transistors remain to be solved, it now appears increasingly likely that organic thin film transistors will find use in a range of commercial, industrial, and military applications. Such applications might include flexible flat panel displays, smart cards, smart inventory tags, supermarket shelf-edge labels, and intelligent sensory arrays.

In this work, we study the transport properties of charge carriers (or holes) in disordered organic semiconductor used as active materials in field effect transistors. Specifically, we investigate the effects of an organic thin film thickness on charge carrier mobility which is the basic parameter for the transport properties.

The rest work of this thesis is divided into four major chapters. The second chapter exposes the basis of charge transport in disordered OFETs. Chapter three deals with a methodology which contain the model and the mathematical techniques used to obtain scientific data. Chapter four presents the result and discussion. In this chapter, all the data obtained are analyzed and discussed in detail. Summary and conclusion of the study are presented in the fifth chapter.

CHAPTER 2

Theory of Charge Transport in Disordered Conjugated Organic Polymers

2.1 A conjugated polymer and its electronic structure

The word polymer originates from the Greek word "poly" meaning many and "mer" meaning part. A polymer is a substance composed of molecules characterized by multiple repetitions of one or more species atoms or group of atoms (constitutional repeating units) linked to each other in the amount sufficient to provide a set of properties which do not vary markedly with the addition of one or a few of the constitutional repeating units.

Each repeating unit is linked to form a monomer. A molecule with only a few constitutional repeating is called an oligomer or small molecule. unlike a polymer, the physical properties of an oligomer vary with the addition or removal of one or a few constitutional repeating units to or from its molecule.

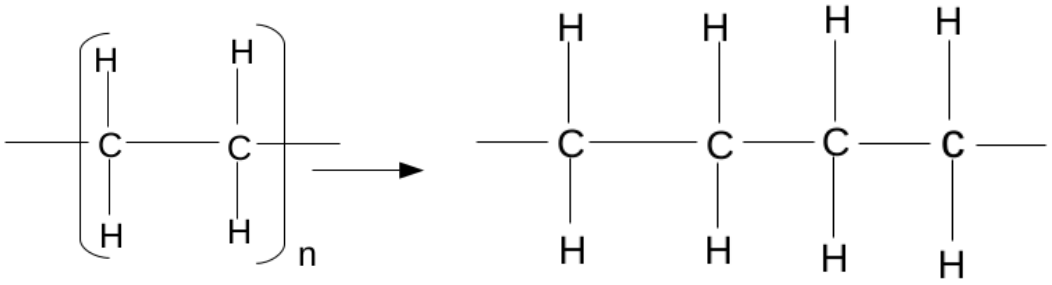
Organic polymer can, in general, be classified as saturated and unsaturated on the basis of the number and type of the carbon valance electron involved in the chemical bonding between consecutive carbon atoms and other neighboring atoms along the main chain of the polymers.

In the case when all the four valance electrons involved in the chemical bonding the polymer are classified as saturated, where as in the case when only three of the

four carbon valance electrons are involved in covalent bonding the polymers are classified as unsaturated. In the first case since all the four valance electrons of the carbon atom are used up in covalent bonds the saturated polymers are insulators, but for the second case there is one more electron left. This electron is called π.

The constitutional repeating units are linked together by covalent bonds to form a polymer, and the atoms of repeating units are also linked by covalent bonds. The process that converts a monomer to a polymer is called polymerization.

The monomer ethane is shown in figure 2.1 (a). The polymer made from repeating units of ethane known as poly(ethane) is shown in 2.1 (b).



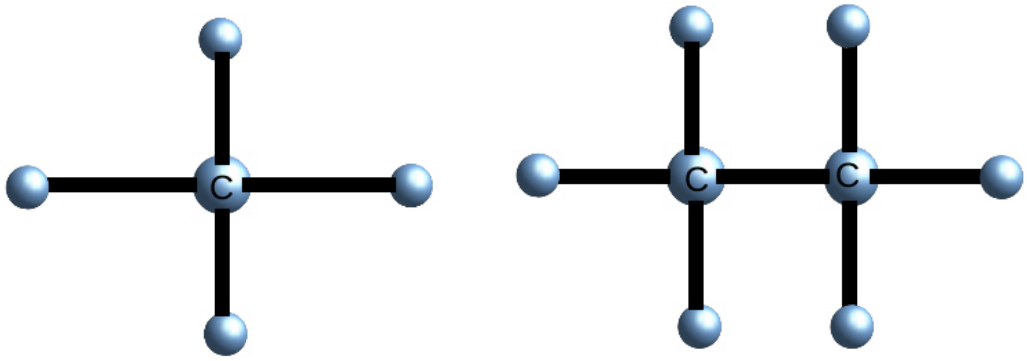
(a) **(b)**

Figure 2.1: Schematic figure of (a) Monomer (ethane) and (b) Polymer (Polyethane)

The π conjugated organic materials are either small molecules or polymers. Ideally, conjugated polymers are infinitely long linear systems regularly built from repeat units containing π electrons extended along the infinite length of the chain.

Organic polymers contain a neutral carbon atom with configuration of $1s^2 2s^2 2p^2$. The electronic properties of the polymer are determined based on the number of valence electrons involved in bonding the carbon atom with other carbon atoms and other elements in the neighbors.

The four electrons in the outer shell have sp^3 or sp^2 configurations. In simple compounds like methane (CH_4) or ethane (C_2H_6) shown in Figures 2.2 (a) and (b)



(a) Methane **(b)** Ethane

Figure 2.2: Schematic figure of (a) Methane and (b) Ethane

one of the 2s electrons is promoted to a 2p and the remaining 2s electron create tetrahedrally equal orbits called sp^3 hybrid. The sp^3 orbitals that we observe in ethane are involved in covalent or σ bonding between carbon and hydrogen atoms.

In the case of sp^2 hybrid configuration only three of the four electrons are involved in covalent or σ bonding and the remaining one electron is involved in π bonding. The σ bond form a plane and determine the structural backbone of the molecule. The remaining one unpaired electron is involved in the formation of a π bond in a p_z orbital is spatially perpendicular to the plane formed by σ bonds.

Each of the unpaired electrons in the p_z orbits of successive carbon atoms along the backbone overlaps with similar electrons in the neighboring and form delocalized π electron system along the polymer backbone.

This electronic delocalization provides a way for an electron mobility along the backbone of the polymer chain. This means that sp^2 configuration is an essential requirement for a polymer to become electrically conductive[5].

The π bond arises from the overlap of the p_z orbitals on both carbon atoms in the neighboring p_z orbitals as shown in Figures 2.3 (a) and (b) [6]. In addition to this, since conjugated polymer repeats their structure in long chains, this structure allows continuous overlap of the p_z orbitals along the length of the chain giving

rise to an extended delocalized p_z conjugated system.

The delocalization along the backbone of the polymer means that π electrons are free to move within the length of the chain or an electron is delocalized.

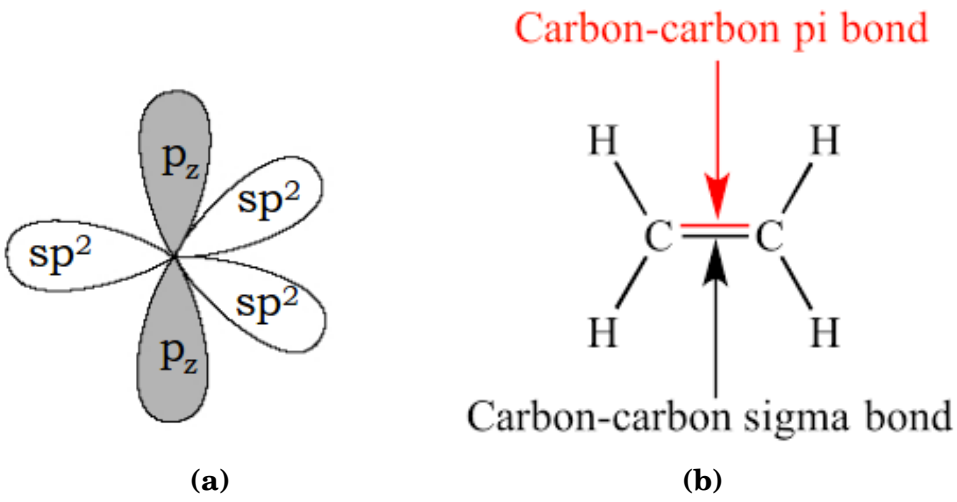


Figure 2.3: (a) sp^2 hybrid orbitals, and (b) P-orbital overlap creating π-bond

The double line between the two carbon atoms shown in Figure 2.3 signifies a double bond which is σ-bond and π-bond. The σ bond is quite strong but the electrons in the π-bonds are less tightly bonded. The π-bonds are easily broken low energy excitations and the electrons involved in the π-bonds are exited into the conduction band. If we consider a single π-bond of any conjugated polymer the two electrons are coupled and hence the energy split into π and π^* bands.

Each carbon atom of any conjugated polymer makes σ-bonds with two adjacent carbon atoms and to one another atom or molecule. Its fourth electron orbits at right angles to the plane formed by σ-bonds and form a π-bond with one of the adjacent carbons. When more double bonds added into the molecule the individual energy level split further. As the number of the double bonds increases, one can talk about a band of energies, that is a band structure.

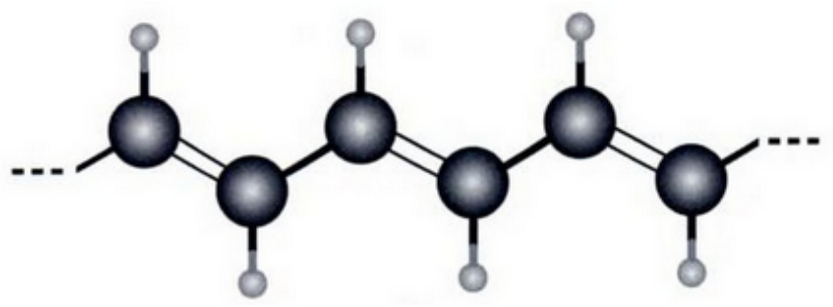


Figure 2.4: Polyacetylene

In long structure, each carbon atom is σ-bonded to two neighboring carbons and one hydrogen atom. Hence we get a polymer known as poly-acetylene as shown in Figure 2.4. In this polymer a single and double bonds alternate. Polymers with such structure are known as conjugated polymers.

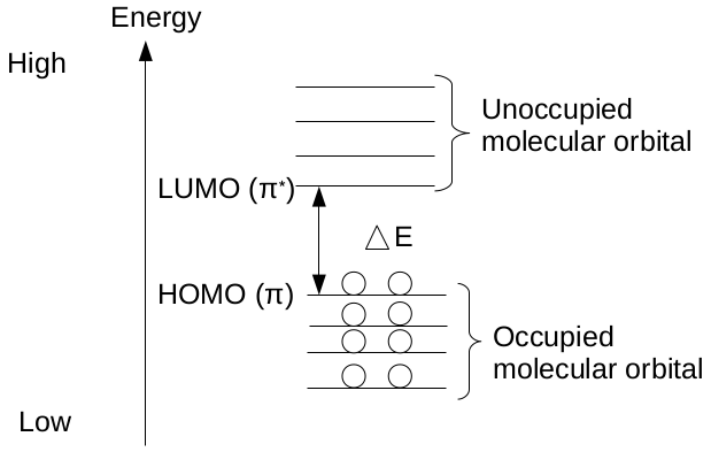


Figure 2.5: Energy difference between LUMO and HOMO

Since each band can hold two electrons per atom (spin up and spin down) the π band is filled and the π^* band is empty as shown in Figure 2.5 [7]. The energy difference between the lowest unoccupied molecular orbital (LUMO) in the π^* band, and the highest occupied molecular orbital (HOMO) in the π band π^* - π energy gap known as band gap (E_g). Consequently, since there is no partially filld bands, conjugated polymers are typically semiconductors. Under normal condition the lower band is fully occupied, the higher band is empty as shown in Figure2.5. Therefore to get free charge carriers in π band and/or π^* band electronic excitation is required for a molecule that contains π-electrons. These excitations are possible with a modest amount of energy, typically 1eV to 3eV[8].

In disordered organic semiconductors polymers, conductivity proceeds via hopping of either electron within a manifold of lowest unoccupied molecular orbital (LUMO) or holes within a set of highest occupied molecular orbitals (HOMO). Both LUMO and HOMO manifolds are characterized by random positions and relatively broad (Gaussian) energy distributions of hopping sites[9].

As described above there are no free charge carriers in a conjugated polymer under normal conditions. Thus free charge carriers are introduced either by doping or by shining it with light or by injecting from metal contacts. In this study, we introduce the charge carriers (or holes) from metal contact by field effect method to the active material (semiconducting polymer thin film) used in field effect transistor (FET) device. The number of free charge carriers (density) depends on the magnitude of the gate voltage.

In this work, we have studied the transport behavior of the charge carriers with the applied electric field along the lateral direction of the film for different film thickness and different charge carrier densities. Specifically, the mobility of charge carriers as a function of an applied electric field along the length of the film is investigated numerically using kinetic Monte Carlo approach for various thickness of the active material and also for different values of the gate voltage. Our work is compared with previous work[10].

2.2 Charge Transport in Disorder Organic Semiconductors

In inorganic semiconductors, the morphology and electronic structure is generally characterized by their strong covalent and ionic bonding between atoms in the lattice. Bloch's theorem is a direct consequence of the periodicity and describes the electrons and holes by wave functions which are extended in space.

A chain of conjugated polymers is held together by strong covalent bonds. On the other hand, the force that exists between molecular chains in a film is a week van-der-Waals attraction. Since it has flexibility character the molecular chains of the film will have the structure of unstirred boiled spaghetti.

Consequently, this flexibility nature together with other chemical defects restricts the length of each chain of conjugated polymers in a film not to stretch indefinitely. Instead, it makes twists or kinks that subdivide the polymer of the same physical chain into a number of conjugated segments and separate them. Also, these twists or kinks disrupt the π bonds and cause each segment to behave like a separate entity, and the molecular film to be considered as a collection of distinct molecular sites. The mean length of these conjugation segments is known as a conjugation length.

The absence of the ordered atomic structure in organic semiconductors necessitates a different theoretical approach. In inorganic semiconductors the charge transport can easily take place through a strong exchange interaction of overlap atomic orbitals in closed-packed structure, whereas in organic semiconductors the bonding between molecules is mainly due to Van der Waals forces and is therefore rather weak, and also the overlap of molecular electron exchange is small.

This implies the transport bands in molecular solid, i.e. valence and conduction bands are narrow. As a consequence, the mean free paths of charge carriers are of the order of the lattice spacing. This renders coherence effects in transport unimportant except at low temperatures. Another consequence of weak inter-molecular interactions is a relatively easy formation of disordered structures, giving rise to the formation of electronic localized states in the band gap, capable of localizing charge carriers.

This means that the polymer chains can not be aligned over their wide length due to this disordered defect and as a result the delocalization length of a π-electron cloud is limited to a definite conjugation length. These conjugation length

segments, bounded by an energy barrier created by the defects or kinks, have random distributions. The distribution of segment length results in the distribution of electron states, and the polymer chains are not aligned with each other over their whole length, but can align only in small crystal regions.

The polymer chains may either extend through a number of crystalline regions or may be folded back on themselves within these regions. In either case, ordered crystalline are interconnected by amorphous regions.

These different local arrangements modify the energies of the conjugated segments because of the variation of the electron polarizability and of local dipole interactions between neighboring chains.This effect, combined with the distribution of segment lengths, broadens the electronic density of states, and because of these electronic conduction occurs by hopping of the carriers from one localized site to another.

In real molecular solids, there are a lot of irregularities which arise from defects in the structure. Therefore, the polarization energies are dispersed. The dispersion of polarization energies influence the energetic distribution of electron states or density of states (DOS) which can be described by a Gaussian distribution[11].

$$g(\epsilon) = \frac{N}{\sqrt{2\pi}\epsilon_o} exp\left[\frac{\epsilon^2}{2\epsilon_o^2}\right] \tag{2.1}$$

The DOS in the mobility gap of some disordered organic materials, and disordered inorganic materials are described by exponential distribution

$$g(\epsilon) = \frac{N}{\epsilon_o} exp\left[\frac{\epsilon}{\epsilon_o}\right] \tag{2.2}$$

where N is the concentration of the site, ϵ_o is the energy scale of the DOS, and ϵ is the energy[12].

A thorough understanding of basic transport mechanisms of charge carriers in organic disordered based electronic devices is crucial to increase the efficiency of the devices apart from academic interest. It is described by the applied electric field-induced directional velocity component (or average drift velocity), v_{av}, of the

mobile charge carriers, which is associated with a current density j

$$j = envav, \tag{2.3}$$

where e is the electronic charge unit and n the local charge carrier density. This velocity v_{av} is directly proportional to the applied electric field F provided that the field is not too high. This relation is written as

$$v_{av} = \mu F, \tag{2.4}$$

where μ is defined as the charge carrier mobility. It is a material specific parameter and plays a fundamental role in charge carrier transport.

Charge transport in semiconducting polymers requires charge carriers motion both along single molecule as well as jumping from molecule to molecule which is often described as a hopping process through energetically disordered landscape induced by defects, disorder, or polarization. Such a localized state is usually called a site for the charge carrier. Through experimental measurement or computational studies, charge transport between molecules has been shown to be several orders of magnitude slower than transport along a single molecule.

Thus, charge transport is limited by the rate of charge carriers moving between molecules. This transport rate depends heavily on orbital overlap and coupling between adjacent molecules as well as the tendency for a charge carrier to be trapped in the energetically disordered landscape of organic semiconductors.

As inter-molecular interactions are so strongly linked to relative orientation and spacing between adjacent molecules, the micro-structure of organic semiconductors is of decisive importance for their electronic properties.

Nevertheless, in a great number of polymeric organic materials the current theory of conduction is based on assumption that due to weak inter-molecular interaction, charge carriers are strongly localized and variable range hopping is the dominant charge transport mechanism. According to this theory charge transport occurs by

thermally activated hopping through a manifold of localized states with a Miller-Abrahams rate equation[13].

$$\nu_{ij} = \nu_o exp\left(-\frac{2r_{ij}}{\alpha}\right) exp\left(-\frac{E_j - E_i + |E_j - E_i|}{2k_B T}\right) \tag{2.5}$$

Equation 2.5 is often written as

$$\nu_{ij} = \nu_o exp\left(-\frac{2r_{ij}}{\alpha}\right) \begin{cases} exp\left(-\frac{E_j - E_i + |E_j - E_i|}{2k_B T}\right), & \text{if } E_j \geq E_i \\ 1, & \text{if } E_j < E_i \end{cases} \tag{2.6}$$

where ν_o is typical phonon frequency prefactor, T is temperature, α is a localisation radius or an inverse wave function decay constant, r_{ij} is the intersite distance between sites i and j, k_B is Boltzmann constant and E_i and E_j are a charge carrier energies at site i and j, respectively.

In this process a charge carrier either absorbs or emits a phonon for a transition to take place. The concept of variable-range hopping suggests that the rate-limiting step in charge transport is a jump of equilibrated carriers, occupying deeper states, to shallower sites that play a role of transport states.

According to the Miller - Abrahams rate equation shown above, the carrier jump rate decreases with increasing both the distance and energy difference between starting and destination sites. A combination of the distance and energy difference that provides the highest jump rate is determined by the temperature, the carrier localization radius and the shape of the electron density of state (DOS) distribution.

Transport energy of hopping in a Gaussian density of state distribution was studied by Bassler [11] employing Monte Carlo simulation techniques. In the case of weak intersite coupling relevant for organic systems it was found that there is a broad distribution of transport energy values and that its maximum decreases with decreasing temperature in qualitative agreement with the concept of variable-range hopping. Both Monte Carlo simulation and analytic consideration have shown that a carrier will most probably jump from a currently occupied state to

a hopping site that belongs to the energy level known as transport energy level.

In order to describe the charge-carrier transport in disorder organic semiconductor, many models have been developed[]. Among these models, the Gaussian disorder model (GDM) exerts a profound infulence[11]. According to this model the on site energies are drawn randomly from a Gaussian type energy distribution, and the charge carriers conduction takes place by hopping between localized sites which is governed by the Miller-Abrahams rate equation.

The rate at which hopping of each charge carrier from an occupied site to an empty site occurs is related to the conductivity or charge carrier mobility of the materials [14][15]. The rate equation described above is the same as $W_{i,j}$, the transition rate for hopping from site i to j, that we observe in the stedy state master equation described bellow.

$$\sum_{j \neq i} [W_{i,j} p_i (1 - p_j) - W_{j,i} p_j (1 - p_j)] = 0 \tag{2.7}$$

where p_i is the probability that site is occupied by a charge carrier and the factor $1 - p_i$ accounts in mean field approximation, for the fact that only one carrier can occupy a site, due to the high coulomb penalty for the presence of two or more carriers.

The most famous analytical result for variable range hopping (VRH) was derived Mott[16][17]. He argued that a characteristic electron transition is from a state with an energy just bellow the Fermi energy to a state with an energy just above it. Only arround the Fermi energy are there both occupied and unoccupied states available. Furthermore, if the energy difference is too large, as it would be if one of the states had an energy far from the Fermi level, the transition rate will vanish according to equation (2.6).

VRH is more general regime of hopping transport which is valid at low temperature. But the tunneling probability of the transitions are taken into account, which means that a spacially near neighbor may be discarded for a neighbor that is closer

in energy[18][19]. This is illustrated in Figure 2.6. While this regime adds a level of complexity to the model, analytical solutions still exists for several choice of the DOS.

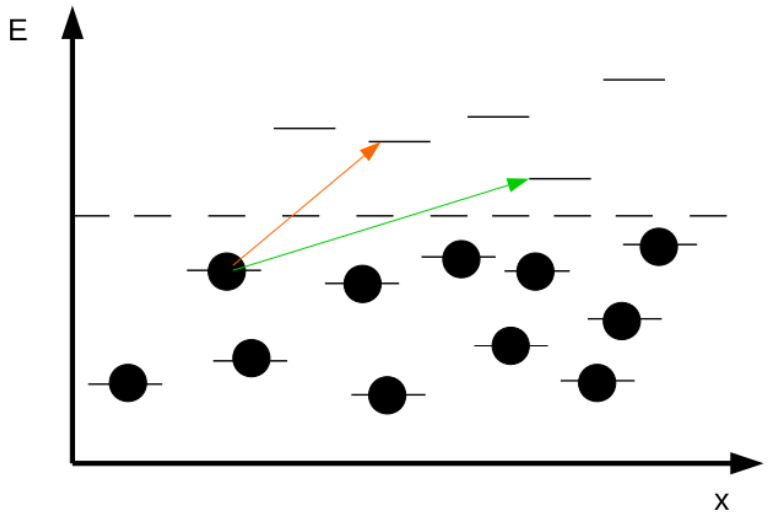


Figure 2.6: VRH hopping model. Acharge carrier (black circle) might choose a site far in space (green arrow) over the nearest neighbor (red arrow), when the energy difference to the latter is too high.

Apart from this random contribution, the energy difference in equation (2.5) contain two contributions.

1. The Columb interaction energy with all other charges, including the gate charge.

2. An electrostatic contribution $-eFR_{ijx}$ due to an electric field F along the length of the film due to source drain bias, and e is the unit charge.

2.3 Charge Carrier Mobility

The mobility describes the response of a charge carrier to an applied electric field. It is defined as the magnitude of the velocity of the charge carrier, usually called the drift velocity, v_d, divided by the magnitude of the electric field F. This definition is valid for both electrons and holes and makes the mobility a positive quantity.

$$\mu_e = \frac{v_d}{|F|}, \qquad \mu_h = \frac{v_d}{|F|} \tag{2.8}$$

where μ_e and μ_h are mobility of electron and hole, respectively. If the applied electric field is small, the charge carrier transport may be better described as a diffusive process than as drift. Due to diffusion, even without an electric field, the charge carrier will pass through the system as long as it is finite. In that case the mobility is better described by the Einestine formula

$$\mu = \frac{eD}{k_B T}, \tag{2.9}$$

where, k_B is Boltzman constant, e is elementary charge and T is temperature. Charge carrier transport is determined by a broad distribution of mobilities. The fact is due to the random nature of the charge carrier transport in an energitically and spatially disordered enviroment[20].

In the absence of an external electric field, charge carriers move randomly within a material with no net drift in any direction. When an external uniform electric field, F is applied, the charge carriers begin to move in the direction of F, and the average drift velocity, v_d, of a charge carrier as it moves through the material in the direction of the field F can be written as

$$v = \frac{L}{\langle t \rangle} \tag{2.10}$$

where $\langle t \rangle$ is the average time taken for a charge carrier to change its position by L[21]. Here mobility can be calculated numerically by determining the the average distance that each charge carrier travel along the field direction and the time taken during this change of position using kinetic MC approach based on equation (2.5)

$$\langle t \rangle = \int t p(t) dt$$

Consequently, the stochastic average of the mobility $\langle \mu \rangle$ is given by

$$\langle \mu \rangle = \frac{L}{F} \int \frac{1}{t} p(t) dt = \frac{L}{F} \left\langle \frac{1}{t} \right\rangle \tag{2.11}$$

2.3.1 Mobility calculation in an organic field effect transistors (OFETs)

In electronic devices such as OFETs a knowledge on the basic transport mechanism may help to increase transport efficiency. Since charge carrier mobility is one of

the basic transport parameters[22] that varies with the material we will calculate the charge carrier mobility of organic thin film which is the active material in the device.

The numerical method for modelling a charge transport with respect to distribution of localized states (DOS) in disordered solids are based on stochastic Monte Carlo method. The inputs parameter of the model are the density of charge carriers that depend on the gate voltage, the thickness of the film, the applied electric field along the lateral direction, and the width of the DOS distribution.

Using a model, the influence of DOS to transient photo-conductivity was examined. It was shown, that the traps in distribution of localized state have the predominant influence on the transient photo-conductivity of disorder solids. Thus, the transient photo-current reflects the DOS can be used with advantage for their determination. For this purpose a post-transient photo-current analysis method was adapted.

The method is based on Fourier transform of the transient photo-current. Based on this transform a numerical procedure for the evaluation of DOS was built. Using the method and numerical modeling it was demonstrated that the post-transient analysis method is suitable for reconstruction of DOS from transient photo-current in organic materials. The accuracy of post-transient analysis method in the determination of energy position and concentration of localized states was examined with favorable results for experimental work.

The OFETs is routinely used as a test structure for extracting mobility in addition to being a key element in circuits. The following therefore describes density of mobile charge carriers in the channel.

$$Q_{mob} = C_i(V_{GS} - V_{th}) \tag{2.12}$$

where C_i is capacitance of the insulater per unit area. The areal density of charge carriers ($\frac{C}{cm^2}$) induced at a given position x along a channel is proportional to the voltage difference

$$V_{GS} - V(x) \tag{2.13}$$

therefore equation (2.12) becomes

$$Q_{mob} = C_i \left(V_{GS} - V_{th} - V(x)\right) \tag{2.14}$$

Assuming that, under the external field F the drift dominate the channel, then diffusion and gate leakage can be neglected (i.e. only consider the movement of charge carriers due to the applied field). The current in the channel I_D is then proportional to the width of the channel, W, the density of mobile charge, Q_{mob}, the electric field F at position x, F(x), and the mobility of the charge carriers due to the applied electric field, μ, can be formulated as

$$I_D = W\mu QF(x) \tag{2.15}$$

where

$$F(x) = \frac{dV}{dx} \tag{2.16}$$

$$\mu = \frac{v}{F} \tag{2.17}$$

where μ is the mobility given in ($\frac{cm^2}{V.s}$). Now, substituting equation equation (2.14) and equation (2.16) into equation (2.15) to yield

$$I_D dx = W\mu C_i \left[V_{GS} - V_{th} - V(x)\right] dV \tag{2.18}$$

and integrating over the potential difference range between the source and drain, i.e. the channel length, L, gives

$$\int_0^L I_D dx = W\mu \int_0^{V_{DS}} C_i \left[V_{GS} - V_{th} - V(x)\right] dV(x) \tag{2.19}$$

then

$$I_D = \frac{WC_i}{L}\mu x \left((V_{GS} - V_{th}) \times V_{DS} - \frac{{V_{DS}}^2}{2} \right) \tag{2.20}$$

Equation (2.20) crossponds to $0 < V_{DS} < (V_{GS} - V_{th})$, which is the linear regime.

2.3.2 The model

We model the OFETs to consist of a thin semiconductor layer, a gate dielectric, and three electrodes, as illustrated in Figure2.7. The source and drain electrodes are connected to the semiconductors whereas the gate electrode is electrically isolated

from the semiconductor by the gate dielectric which is taken usually as $\epsilon_r = 3$.

In this study, organic transistors are discussed which operate in uni polar p-type accumulation mode. When a negative bias is applied to the gate holes accumulate at the semiconductor-dielectric interface. The accumulated holes form a conducting path between the source and drain electrodes, allowing current to flow. This is the region in which all of the critical charge transportation occurs. The channel is only a few nanometers thick which is about 5-6nm[23][24]. The Charge carriers will also produce an electric field (E_z) that result in introducing the potential along z which is given by ($U_{vg}(\Delta z)$).

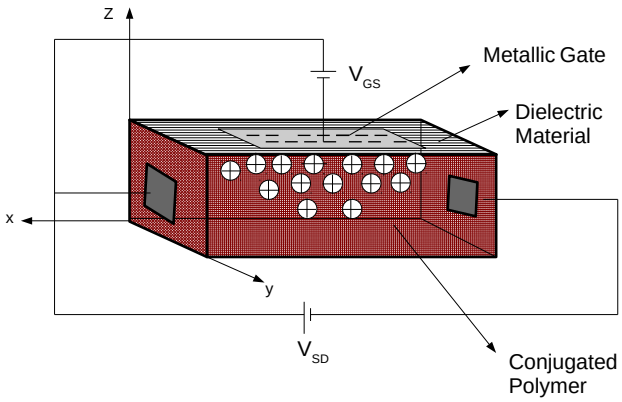


Figure 2.7: Three dimensional box showing when negative voltage (V_g) applied to accumulate p-type charge carriers in the active material.

Now, we can find the potential due to E_z which is $U_{Vg}(\Delta Z)$

$$U_{vg}(\Delta Z) = e \times E_z \times r \tag{2.21}$$

where ΔZ is the change of dimension along Z, V_g is the voltage on the metalic gate, E_z is the field along Z and U_{Vg} is the potential due to gate bias.
But, from equation (2.21) we obtain:

$$U_{vg}(\Delta Z) = a \times E_z \times e \tag{2.22}$$

where a is lattice parameter e elementary charge.
But, from figure 2.7 the electric field (E_z) is given by

$$E_z = \frac{\sigma}{2\epsilon_o\epsilon_r} \tag{2.23}$$

where $\epsilon_r = 3$,$\epsilon_o = 8.854 \times 10^{-12} Fm^{-1}$ which is given in $\frac{Frad}{m}$ and σ is surface charge density but the capacitance of the capacitor can be given by:

$$c = \frac{Q}{V_g} \tag{2.24}$$

dividing both side of equation (2.24) by A we arrive to

$$\frac{c}{A} = \frac{Q}{AV_g} \tag{2.25}$$

where, $\frac{c}{A} = 17nFcm^{-2}$ where $\sigma = \frac{Q}{A}$, substituting equation (2.25) we obtain:

$$C = \frac{\sigma}{V_g} \tag{2.26}$$

$$\sigma = C \times V_g \tag{2.27}$$

Substituting equation (2.27) and equation (2.23) into equation (2.22) we get

$$U_{vg}(\Delta Z) = a \times \left(\frac{C \times V_g}{2\epsilon_r\epsilon_o}\right) \times e \tag{2.28}$$

$$U_{vg}(\Delta Z) = a \times \left(\frac{C}{2\epsilon_r\epsilon_o}\right) \times V_g \times e$$

Now, taking the equation which is in the brace and substituting the constatants

$$\frac{17 \times 10^{-5} Fm^{-2}}{2 \times 3 \times 8.854 \times 10^{-12} Fm^{-1}}$$

then we have

$$0.32 \times 10^7 m^{-1} \tag{2.29}$$

Using equation (2.29) into equation (2.28) we obtain

$$U_{vg}(\Delta Z) = a \times \frac{(0.32 \times 10^7 m^{-1})}{k_B T} \times V_g \times e \tag{2.30}$$

and multiplying equation (2.29) by $\frac{\sigma}{\sigma}$

$$U_{vg}(\Delta Z) = a \times \frac{(0.32 \times 10^7)}{k_B T} \times V_g \times e \times \frac{\sigma}{\sigma}$$

rearrenging the above equation

$$0.32 \times 10^{7} m^{-1} \times V_g \times \frac{ea}{\sigma} \times \frac{\sigma}{k_B T}$$

where $a = 1nm$ is lattice parameter, $\hat{\sigma} = \frac{\sigma}{k_B T} = 4$ which is the morphology of the acive material for 300k and $\sigma = 0.1ev$ therefore equation (2.30) can be written as

$$0.32 \times 10^{7} m^{-1} \times \frac{1.602 \times 10^{-19} C \times 10^{-9} m}{\sigma} \times V_g \times \frac{\sigma}{k_B T} \tag{2.31}$$

$$U_{vg}(\Delta Z) = V_g \times 0.32 \times 0.01 \times \left(\frac{\hat{\sigma}}{\sigma}\right) \tag{2.32}$$

Now, we can calculate the amount of charge (Q) accumlated on the metalic gate using gate voltage

$$Q = CV_g \times length \times width \tag{2.33}$$

$$Q = \frac{17 \times 10^{-9} \times 10^{4} \times 10^{-14} \times V_g F cm^2}{cm^2}$$

$$Q = \left(\frac{17 \times 10^{-9} \times 10^{4} \times 10^{-14} \times F cm^2}{cm^2}\right) \times V_g$$

$$Q = \left(17 \times 10^{-19} F\right) \times V_g \tag{2.34}$$

Thus we can find the number of paticle (N_p) accumlated on the metalic gate

$$N_p = \frac{Q}{e} \tag{2.35}$$

Substituting equation (2.35) into equation (2.34) one can find:

$$N_p = \left(\frac{17 \times 10^{-19} F}{1.602 \times 10^{-19} C}\right) \times V_g$$

$$N_p = 10.625 \times V_g \tag{2.36}$$

Now in our case we consider by taking the values $V_g = 5V$, $N_p = 53$ and $V_g = 10V$, $N_p = 106$.

In Figure 2.7 most of the charge carriers are found in the first mono-layer and the charge distribution decay rapidly with increasing distance into the organic semiconductors. The above situation of charge carriers transport is governed by the following effects[25].

(i) state - filling effect

Under this effect we consider the charge carrier occupies a larger volume which decreases charge carrier density so that the decrease in charge carrier density has the tendency of decreasing the carrier mobility.

(ii) Coulomb interactions

Once the charge occupies a larger volume, the Coulomb interaction between the charge carrier is reduced and this has the tendency to increase carrier mobility.

(iii) Availability of new path way

When other monolayers are added, many more pathways become available for a charge carrier to move from source to drain electrode. This also has the tendency to increase the charge carrier mobility.

CHAPTER 3
Computational Techniques and Methods

For the deal of charge transport properties in OFETs, there are many kinds of simulation techniques can be considered. But, the most widely preferable related to this particular work and special for atomic and sub-atomic level modeling are Monte-Carlo (MC) and molecular dynamics (MD).

Montecarlo (MC) simulation can be carried out for repeated random sampling for statistical analysis to compute the result. This method of simulation is very closely related to random experiments, experiments for which the specific result is known in advance.

The GDM model is treated by MC simulation technique, in which charge transport is described as an incoherent random walk. this idea of MC simulations is that the physical system described with the evolution of probability density function. The evolution in GDM described with Miller-Abrahams rate equation (2.3). The initial probability density function is described by the spatial distribution and energetic distribution of charge carriers. We assume hopping of charge carrier from site i to site j was performed on the basis of the probability that a carrier jumps from the present site i to site j given by

$$p_{ij} = \frac{\nu_{ij}}{\sum_{i \neq j} \nu_{ij}} \tag{3.1}$$

where ν_{ij} is the transition rate from site i to j and from equation (3.1) one can obtain hopping time τ_k for the k^{th} in the simulation as follows

$$\tau_k = \frac{-log(U_r)}{\sum_{i \neq j}^{N} \nu_{ij}} \tag{3.2}$$

where U_r is the random number drawn from the interval [0,1). Finally, we begin to

record the mobility of the charge carrier using

$$\mu = \frac{v}{F} = \frac{\sum x_k}{F \sum_k \tau_k} \tag{3.3}$$

where μ is the mobility v is the drift speed, F is the electric field applied along x.

3.1 The Metropolis algorithm

The metropolis algorithm can be stated in the context of the simulation of particles as follows

1. Stablish an initial micro-state
2. Make a random trial change in the micro-state
3. Compute $\Delta E = E_{new} - E_{old}$ the change in the energy of the system due to trial change
4. If $\Delta E \leq 0$ accept the new micro-state and go to step 8
5. If ΔE is positive, compute the quantity $w = e^{-\beta \Delta E}$, $\beta = \frac{1}{k_B T}; k_B$ is Boltzmann constant and T is absolute temperature
6. Generate a random number ζ in the interval [0,1)
7. If $\zeta \leq w$, accept the new micro-state otherwise retain the previous micro-state.
8. Determine the value of the desired physical quantities
9. Repeat steps 2 through 8 to obtain sufficient number of micro-state
10. Compute averages over micro-states

3.2 Kinetic Montecarlo Method

Organic semiconductor materials are usually described in the framework of the hopping model in combination with Kinetic Montecarlo (KMC) simulation. The main idea behind KMC is to use transition rates that depend on the energy barrier between the states with time increments formulated so that they relate to the

microscopic kinetics of the system.

In metropolis Montecarlo method we decide to accept a move by considering the energy difference between the state but in KMC method we use rates that depend on the energy barrier between the states.

The idea of KMC is not to compute probabilities $P_i(t)$ explicitly, but to start with some particular configurations, a representative for initial state of the experiment one way to simulate and then generate a sequence of other configuration with the correct probability.[26]

3.2.1 Infrequent event

An infrequent event is characterized by occasional transitions from one state to another, with long periods of relative in-authenticity between this transitions. The infrequent event designation corresponds to a single energy basin, and the long time between transitions arises because the system must surmount an energy barrier to get out from the basin to another as shown below

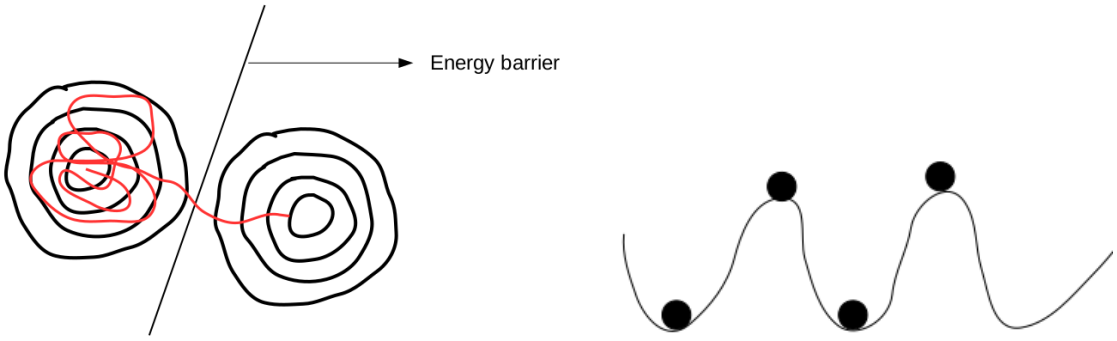


Figure 3.1: Basines with energy barrier

From the above figure, one can recognize that at the bottom of the energy basin the force on every atom or particle of the system is minimum. This defines a particular state i of the system and the geometry at the minimum can be considered as r_i. The system will vibrate about this minimum energy. If the system is heated we still consider the system is in state i if it has not escaped over a barrier.

The important property of an infrequent event system caught in a particular energy basin is that because it stays there for a long time relative to the time of one vibrational period, the system forgets how it got there.

For each possible escape pathway to an adjacent basin, there is a rate constant k_{ij} that characterizes the probability per unit time, that is escape to the state j, and these rate constants are independent of the state preceded state i, each state constants k_{ij} is purely a property of the shape of the potential basin j.

3.2.2 The rate constant and first order process

One of the fundamental ideas behind the entire KMC approach is that during its thermal vibration motion in one of the potential energy surface(PES) basins the system loses the memory of its past history. Also one may assume that this loss of memory occurs continuously so that the system has the same probability of finding the escape path during each short increment of time spent in PES basin. The probability that the system has not yet escaped from state i is given by

$$p_s(t) = exp(-k_{tot}t) \tag{3.4}$$

where p_s is the survival probability and k_{tot} is the total escape rate from the state i, then the probability that the system has escaped after a time t is

$$p(t) = 1 - exp(-k_{tot}t)$$

The probability distribution function per unit time for first escape is

$$\frac{dp}{dt} = \frac{d}{dt}\left[1 - exp(-k_{tot})\right] \tag{3.5}$$

$$p(t) = K_{tot}exp(-k_{tot})$$

The average time for escape τ is just

$$\tau = \int_0^\infty tp(t)dt = \int_0^\infty \left[tk_{tot}e^{-k_{tot}t}dt\right] \tag{3.6}$$

$$\tau = k_{tot}\int_0^\infty te^{-k_{tot}t}dt$$

employing integration by part we obtain

$$\tau = \frac{1}{k_{tot}} \tag{3.7}$$

where

$$k_{tot} = \sum_j k_{ij} \tag{3.8}$$

For each pathway, there is a probability per unit time distribution

$$p_{ij} = k_{ij} exp(-k_{ij} t) \tag{3.9}$$

Assume that all the rate constants are known for each state. Our system is in state i, and we have a set of pathways associated with rate constant $\{k_{ij}\}$. To advance the clock we draw a random time from the exponential distribution for the rate constant k_{tot} once the system is in a new state, the list of pathways and rate is updated, and the procedure is repeated.

$$\int_0^{t'} k_{tot} e^{-k_{tot} t'} dt' = r \tag{3.10}$$

$$- e^{k_{tot} t} + 1 = r \tag{3.11}$$

$$e^{-k_{tot} t} = 1 - r \tag{3.12}$$

$$k_{tot} t = -ln(1 - r) \tag{3.13}$$

substituting Eq 3.7 into 3.13 one can obtain

$$t = -\tau ln(1 - r) \tag{3.14}$$

3.3 Montecarlo Simulation

We model the organic semiconductor as a set of N_z mono-layers stacked on top of each other in the z-direction to form a regular three-dimensional lattice. Each mono-layer is modeled as a square lattice of sites with lattice constant a = 1nm, a typical value for organic molecular semiconductors. The vertical distance between the mono-layers is also taken as a. The simulation box then has N_x, N_y, and N_z lattice sites, where N_x, N_y, and N_z are the number of sites in the x, y, and z-direction, respectively. Periodic boundary conditions are taken in the x and y directions[27].

We performed Monte Carlo simulations for charge transport in three-dimensional square lattices of 100 $\times$ 100 $\times$ N_z sites for different values of N_z. The thickness

of the gate dielectric is taken to be the typical 200nm, which is a typical value for OFETs. Other values of this thickness would simply imply a scaling of the gate voltage. For all the calculations we assumed a temperature of T = 300k. We start with an empty lattice and fill it with a prescribed number of charges that is determined by the applied gate bias. We assume the charges to be holes, which means that a negative gate voltage is taken. After filling, hops of these charges are chosen with weights determined by the hopping rates equation (2.3). Hopping times are chosen from an exponential distribution with an inverse decay time equal to the sum of all possible hopping rates. An applied source-drain electric field of $F = \frac{\sigma}{ea}$ was taken in the simulations, which is well within the linear regime of the charge transport.

If the event's target site was free, the event was executed. Alternatively, if the event was not executable, the charge carrier was allowed to remain in its place and was assigned a new event which was correspondingly in turn placed in the event queue.

1. Charge carriers are randomly placed in the simulation box lattice
2. Each charge carrier is assigned an event, where events are placed into site queue in accordance with their scheduled simulation time
3. First event in site queue is executed if possible, otherwise the corresponding charge carriers location is left unchanged
4. The charge carrier from step 3 is assigned a new event time and destination and placed in the event's site queue. Finally the simulation return to step 3.

CHAPTER 4
Result and Discussion

We start with analyzing charge carriers mobility for different thickness of the semiconductor layer. We also plot the fraction of the total charge carriers mobility in each mono-layer for different layer thickness, for relatively low, V_g = -5V, and high, V_g = -10V, applied gate bias voltage and finally we compare charge carrier mobility for disorder parameter $\frac{\sigma}{k_BT} = 4$, weak and $\frac{\sigma}{k_BT} = 3$, relatively strong in each mono-layer for different thickness layer with temperature value T = 300k in all cases.

4.1 The Effect of Coulomb Interaction on Charge Carrier Mobility

Under this section, we mainly discuss the charge carrier mobility as a function of layer thickness with and without Coulomb interaction. If we increase layer thickness the charge carriers have the tendency to occupy a larger volume which reduces the Coulomb interaction among the charge carriers specifically for disorder parameter given by $\frac{\sigma}{k_BT}$.

4.1.1 Charge carriers mobility with out Coulomb interaction

We plot the charge carrier mobility with out Coulomb interaction as a function of field by varying the thickness layer (N_z) for Figure 4.1(a) N_p = 53 and 4.1 (b) N_p = 106.

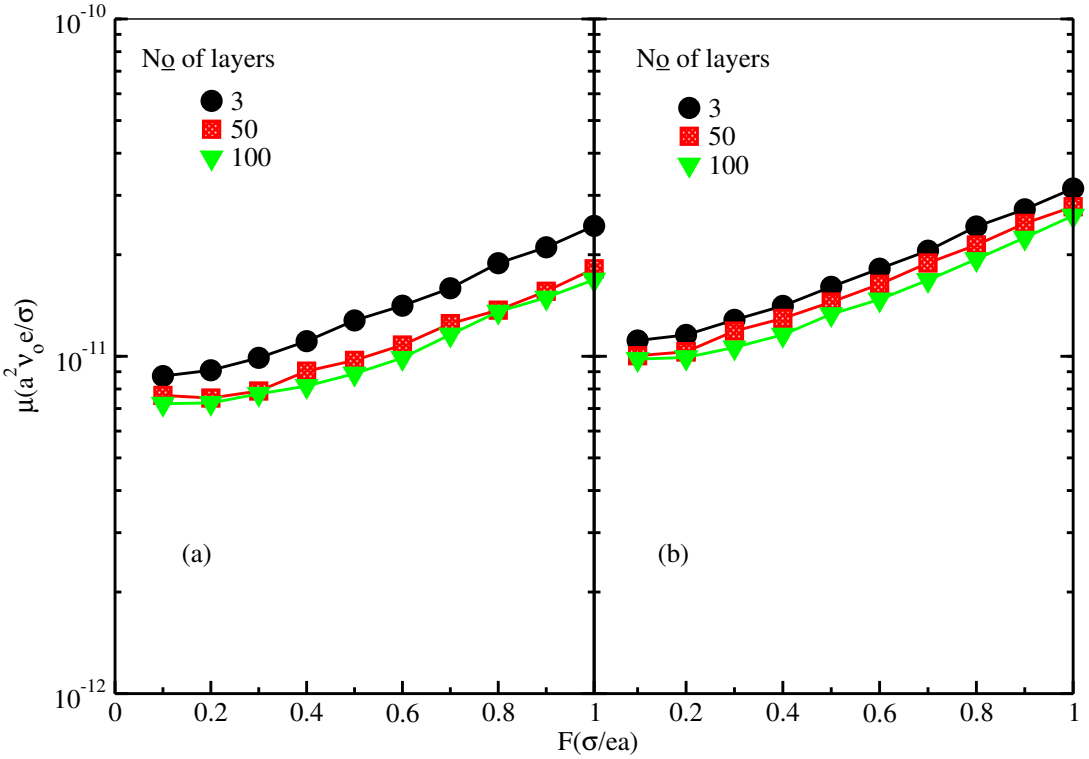


Figure 4.1: Charge carrier mobility varying thickness layer with out Coulomb interaction for (a) N_p = 53 and (b) N_p = 106

As we observed from Figure 4.1 (a) and 4.1 (b) the mobility decrease with increasing layer thickness from the interface where no Coulomb interaction between charge carriers. In this case, the state filling effect is dominant over the availability of new route for the situation of moving away from the interface to occupy larger volume to decrease charge carrier density that in turn decreases the charge carrier mobility. The other important outlook of Figure 4.1 is the number of particles are considered for (b) N_p = 106 the mobility is better than (a) N_p = 53 due to charge carrier density.

4.1.2 Charge carrier Mobility with Coulomb interaction

The effect of Coulomb interaction among charge carriers as a function field especially for increasing layer thickness from the dielectric interface down to the active material. In plot figure 4.2 (a) for N_p = 53 and (b) N_p = 106.

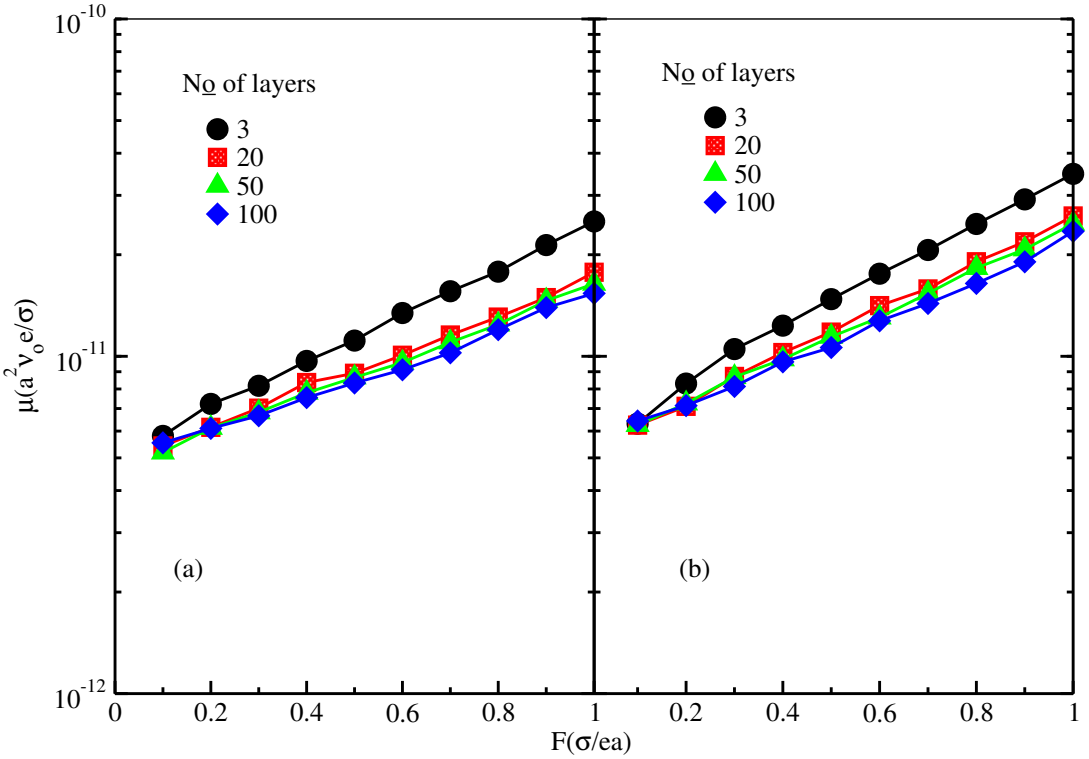


Figure 4.2: Charge carrier mobility varying thickness layer with Coulomb interaction

The plot of Figure 4.2 indicates Coulomb interaction that exists among charge carriers shows monotonically increasing behavior, especially for three layers. This is due to addition of layer thickness make the charge carriers to have a possibility of getting a new route to increase charge carriers mobility. For more layers added the Coulomb interaction and state-filling effect begin to take dominance on new pathway available this result in the decrease of charge carrier mobility relatively.

4.1.3 Charge carrier mobility with and with out Coulomb interaction

In the plot figure 4.3 we basically consider the behavior of charge carriers mobility with and without Coulomb interaction for varying layer thickness from dielectric gate which are displayed in the left panels Figure 4.3 (a), N_p = 53 and 4.3 (b), N_p = 106. Moreover, we tried to compare and contrast the right panel with the left one on the basis of charge carrier density.

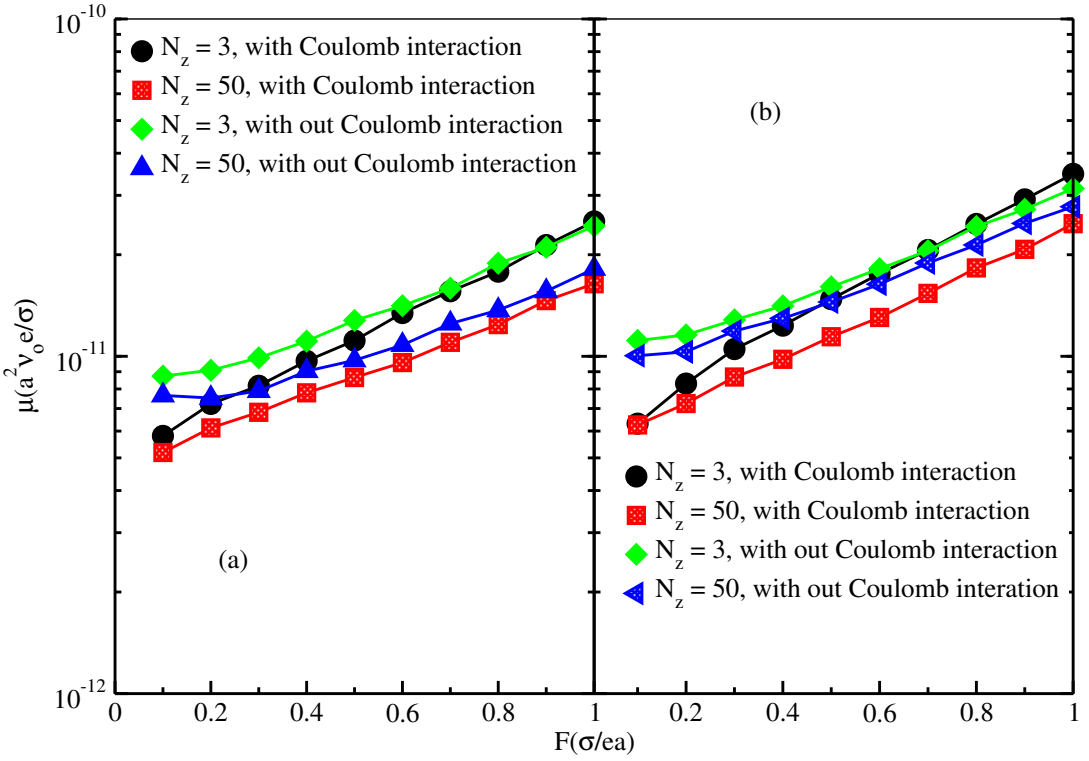


Figure 4.3: Charge carrier mobility with and with out Coulomb interaction in varying layer thickness for (a) N_p = 53 and (b) N_p = 106

In Figure 4.3 the Coulomb interaction among charge carrier in particular between holes is repulsive therefore as the applied field becomes more strong the repulsive interaction becomes more strong that enhance charge carrier mobility.

4.2 Charge carrier mobility as a function of gate voltage

The total number of charge carriers in the active material corresponds to the magnitude of the gate voltage applied. In this section we investigate the charge carrier mobility by fixing layer thickness to N_z = 3, for gate voltage, V_g = -5V, and V_g = -5V that is directly related with the number of particle given by N_p = 53, and N_p = 106 respectively.

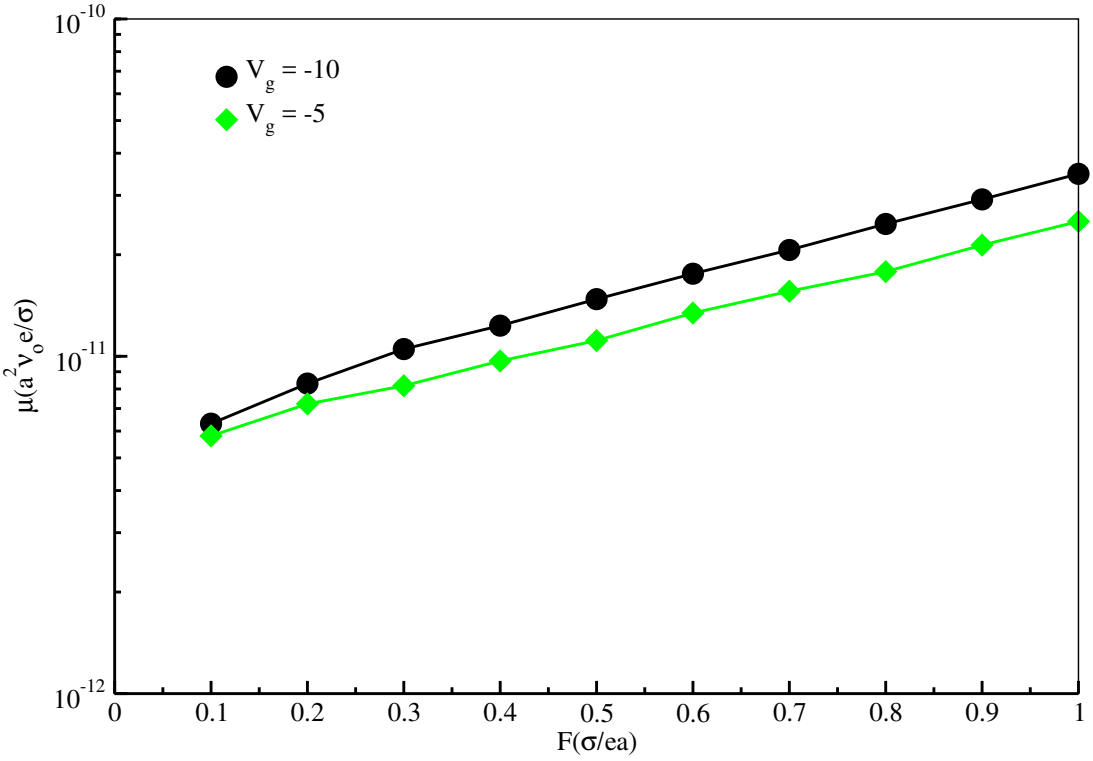


Figure 4.4: Charge carrier mobility for varrying gate voltage

The plot Figure 4.4 shows that for high gate voltage applied on the metallic gate contact will also increase the mobility of the charge carrier between the source and drain electrode this is because we have more charge carrier that is involved in the drift between the two electrodes so than for increasing charge density will increase the charge carrier mobility. This is due to for higher density relatively the charge carriers will geometrically confine in a very small space to intensify Coulomb interaction between charge carriers especially for the strong applied field as in Figure 4.4 one can identify that charge carrier for higher density monotonically increasing relatively than lower density.

4.3 The Effect of Coulomb Interaction on Mobility in Varrying Layer Thickness

The effect of Coulomb interaction on charge carrier was addressed in previous sections, but under this section, our insight observation is Coulomb interaction to compare two dimensional (2D) with three dimensional (3D). The plots are given

in Figure 4.5 and 4.6 are organized in increasing layer starting from the first dielectric layer beneath the active material.

4.3.1 Charge Carrier Mobility with out Coulomb Interaction

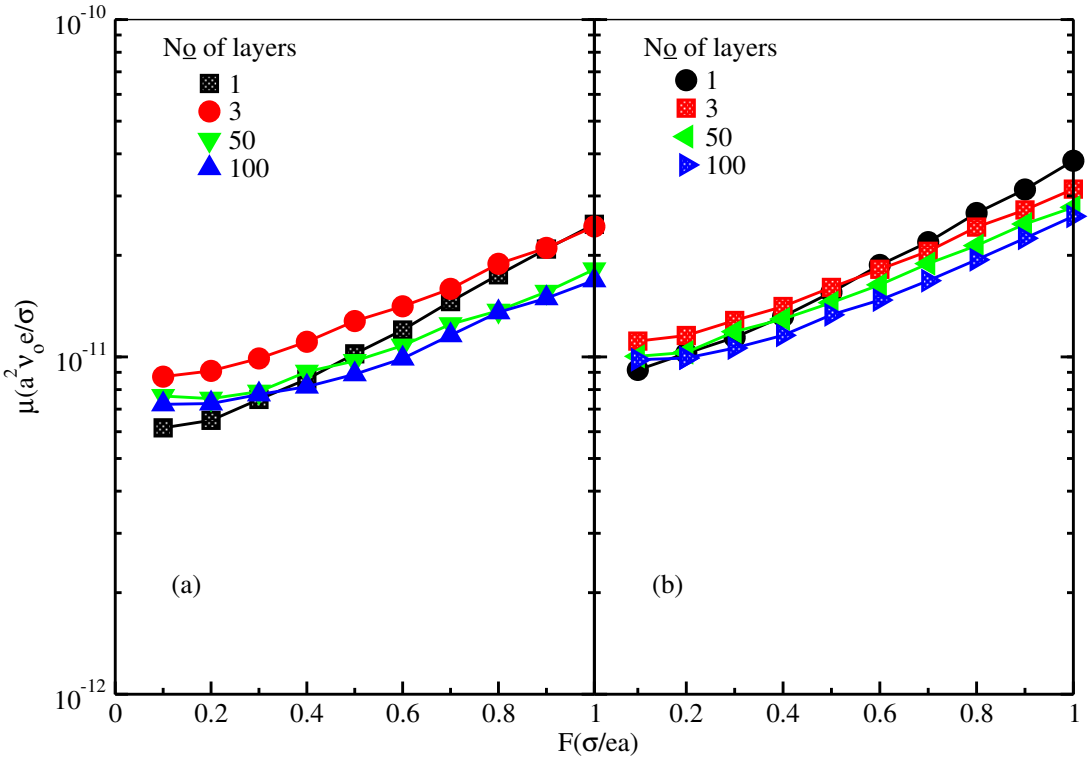


Figure 4.5: Charge carriers with out Coulomb interaction used to compare 2D with 3D for (a) N_p = 53 and (b) N_p = 106

For plot Figure 4.5 (a) and 4.5 (b) it is true that charge carrier mobility shows increment especially up to the third layer which finally appears to be coinciding with the first layer as the electric field becomes strong as in Figure 4.5 (a) but for 4.5 (b) we can see for strong field the mobility in the first layer overreach even the third layer on account of state-filling effect dominating availability of new pathways since charge carrier has a tendency of occupying a larger volume to decrease charge carrier density that decreases charge carrier mobility.

4.3.2 Charge Carrier Mobility with Coulomb Interaction

In Figure 4.6 Coulomb interaction is considered beginning from the gate dielectric interface down to active material showing a property that varies charge carrier mobility as a function field.

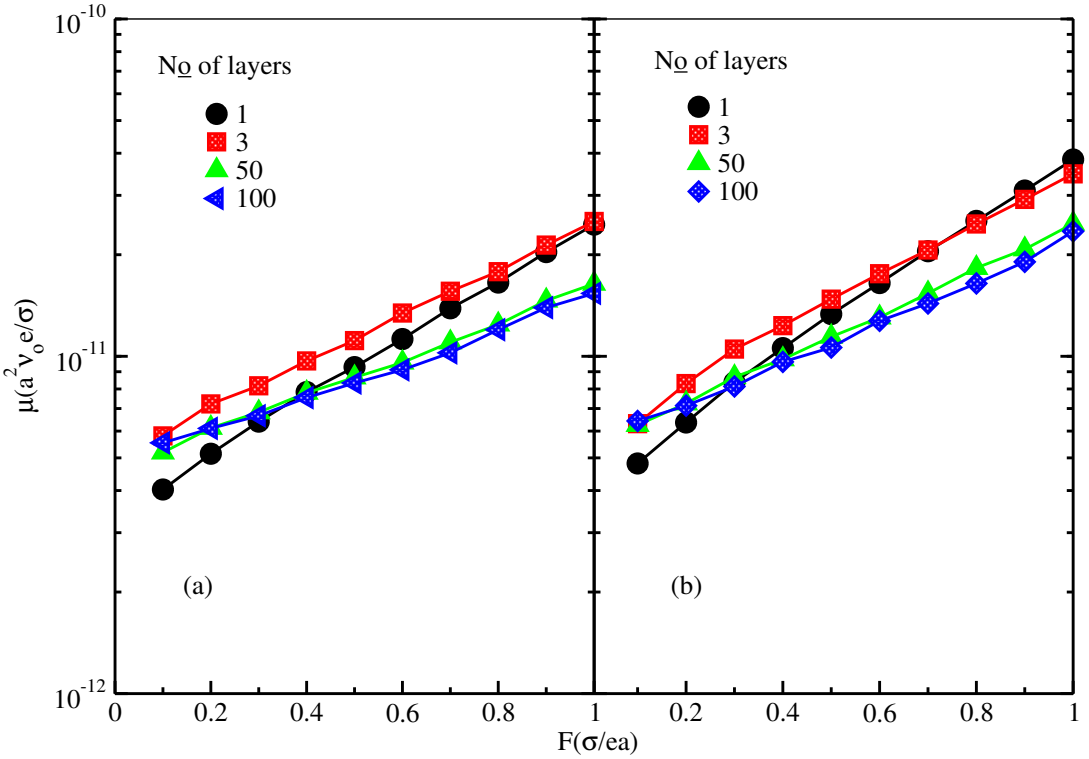


Figure 4.6: Charge carriers with Coulomb interaction used to compare 2D with 3D for (a) N_p = 53 and (b) N_p = 106

Now, considering without Coulomb interaction for fig:4.6 (a) and 4.6 (b) regardless of the difference of the number of particle we are going to look the three effects specifically up to the third layer, as we increase layer thickness new pathway is available for charge carrier that increases charge carrier mobility and also the Coulomb interaction decrease because the charge carriers can occupy larger volume but in state-filling effect charge carrier mobility decrease as the charge carrier occupy larger volume due to the decrease of charge carrier density.

Winding-up from plot Figure 4.6 (a) and Figure 4.6 (b) one can understand that charge carrier mobility shows increment especially up to the third layer but when we extend layer thickness beyond the third layer charge carrier mobility are not good enough and this is due to for increasing layer thickness charge carrier density will tend to decrease charge carrier mobility.

4.4 The Effect of Disorder Active Material on Charge Carrier Mobility for Different Layer Thickness

In plot 4.7 we study how does disorder of active material affect the charge carrier mobility as a function of field for $N_p = 53$.

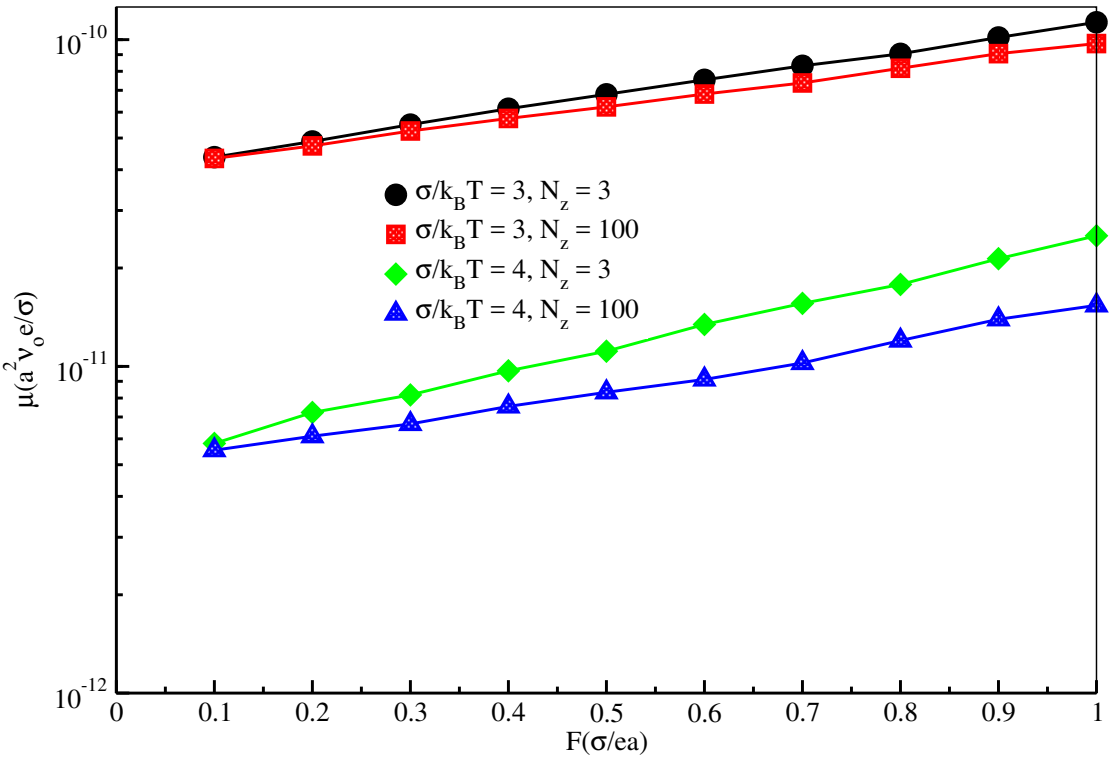


Figure 4.7: The variation of charge carrier mobility as a function of field for different layer thickness by considering morphology of the active material

The plot of Figure 4.7 reveal that charge carrier mobility monotonically increasing for both $\frac{\sigma}{k_B T}$ in spite of layer the difference between weak disorder given by $\frac{\sigma}{k_B T}$ = 3 and strong disorder $\frac{\sigma}{k_B T}$ = 4 relatively is pronounced this attributable for energy band width given by σ. Since mobility of the charge carriers can easily be correlated with σ using $\mu = \frac{a^2 \nu_o e}{\sigma}$. Therefore we identify that for strong disorder the charge carrier mobility much less than that of weak disorder.

CHAPTER 5
Summary and Conclusion

We investigated the effect of increasing the magnitude of gate bias and Coulomb interaction of charge transport in OFETs. The study carried out using Montecarlo simulations of hopping transport in the organic semiconductor which is modeled as a regular array of sites consisting of a layer on the bottom of the gate dielectric. we also examine the influence of varying the thickness of a semiconductor layer and the gate bias.

We identified three effects that determine the dependency of charge carrier mobility on the semiconductor layer thickness: state filling effect, Coulomb interaction, and the availability of charge transport pathways. The state filling effect, which has a tendency of decreasing charge carrier mobility as the charge carrier density decreases due to the larger volume. on the other hand coulomb interaction between the charge has the tendency to decrease the mobility with increasing density. The availability additional pathway for transport upon increasing the thickness of the semiconductor layer also has the tendency of increasing the charge carrier mobility.

It is the competition among these three effects that determines whether the charge carrier mobility increase or decrease with increasing semiconductor layer thickness. We found for disorder parameter $\hat{\sigma} = 4$ charge carrier mobility increase especially for the third and fifth layer for this particular study.

We also found that morphology of the active material can affect the charge carrier mobility in such a way that for disorder parameter given in $\hat{\sigma} = 3$ is much better than disorder parameter given in $\hat{\sigma} = 4$ therefore strong disorder is better for

charge carrier mobility than weak disorder especially in our case.

We confirm that by switching off hopping in the direction perpendicular to the active material in the simulation, we conclude that hopping between mono-layers is a crucial element of charge transport in OFETs. Our final conclusion is that charge transport in OFETs is essentially a three-dimensional process.

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DECLARATION

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MSc Thesis

I the under signed declare that the thesis is my original work and no part of it can be claimed as an intellectual property of anybody else except me and my advisors.

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