Appendix A

Electrons in Organic Molecules

Details about the different types of electrons depending on the degree of localization are described in Fig.A.1. Generally, organic molecules have four different types of electrons\[129\], which may be categorized in the following way:

1. **Core electrons** are essentially localized on a specific nucleus. Useful information about these electrons can be acquired by measuring variations in core binding energies by x-ray photoelectron spectroscopy.

2. **σ Electrons**: are localized between two bonded nuclei.

3. **n Electrons**: are associated with heteroatoms (atoms other than C and H, such as O, N, metal ions... etc.). These are not the bonding electrons but affect the reactivity of molecules.

4. **π Electrons**: are associated in bonding but form weaker and often less-localized bonds than the internuclear σ bonds. The compounds possessing π electrons are called unsaturated compounds. The molecular orbital defining π electron distribution are orthogonal to those which define both σ and n electrons.

![Diagram of different types of electrons and ground state electron distribution](image)

Figure A.1: *Different types of electrons and ground state electron distribution.*
Appendix B

Poole-Frenkle Field Dependent Mobility

The hopping probability of the charge carriers from an energy level in one molecule to an energy level in an adjacent molecule higher by an amount $\Delta$, is

$$ P \propto \exp\left(-\frac{\Delta}{k_B T}\right) \tag{A.1} $$

where $k_B$ is the Boltzmann's constant and $T$ is the temperature. The effect of the electric field is to assist the hopping process by reducing the energy barriers($\Delta$). Consider a general form of the potential $-C/r^n$ existing between the molecules, where $C$ is a constant and $r$ is the radial distance from the charged site. The resultant potential under an electric field $F$ can be given by

$$ U(r) = -C/r^n - eFr \tag{A.2} $$

The maximum of this potential (obtained by $dU/dr = 0$) occurs at $r = r_p$, and is given by

$$ r_p = (nC/eF)^{1/(n+1)} \tag{A.3} $$

The maximum potential can be given by

$$ \Delta U_p = (C/r_p^n) + eEr_p \tag{A.4} $$

From the above two equations,

$$ \Delta U_p = 2(eE)^{n/(n+1)}(nC)^{1/(n+1)}[1 + 1/n] \tag{A.5} $$

Hence the electric field dependence of the mobility is then

$$ \mu(F) \propto \exp\left(F^{n/(n+1)}\right) \tag{A.6} $$

For Coulomb potential

$$ U(r) = (1/4\pi \varepsilon_s)(e^2/r) \tag{A.7} $$

where $n = 1$, $C = e^2/4\pi \varepsilon_s$. Now here the barrier reduction is

$$ \Delta U_p = (e^3F/\pi \varepsilon_s)^{1/2} \tag{A.8} $$
This is the \( \exp(\sqrt{F}) \) dependence of mobility as predicted by Poole-Frenkle[44]. The mobility of the charge carriers for amorphous materials is described by Poole-Frenkle, as a stretched exponential field dependence,

\[
\mu(F, T) = \mu(0, T) \exp \left( \gamma(T) \sqrt{F} \right)
\]  

(A.9)

where, \( \mu(0, T) \) is the zero field mobility and \( \gamma(T) \) describes the field activation of the mobility. Both \( \mu(0) \) and \( \gamma \) have the temperature dependent factors. \( \exp(\sqrt{F}) \) dependence of mobility have been observed in several experiments. Also a numerous theoretical attempts have been made to provide \textit{ab initio} explanation of this almost universally observed[11, 48] proportionality between \( \ln \mu \) and \( \sqrt{F} \) in wide class of disordered materials.
Appendix C

Vacuum Deposition Technique (VDT)

A schematic diagram of the vacuum deposition system is shown in Fig. A.2. Organic materials with high melting point can be evaporated by heating in vacuum, and can be deposited as stable thin films by condensing the vapor on substrates. This vacuum deposition technique has the advantage of depositing a desired film thickness, even in nanometer range, in the clean environment of high vacuum. Although the vacuum deposition is widely used for film preparation of inorganic materials in industrial scale, it has sparsely been applied for organic materials, since the solution-based methods are considered to have higher throughput and cost performance. On the other hand, recent advancement of organic light emitting diode was made possible by constructing multi-layered structure by vacuum deposition method. It indicates that the physical vapor deposition might be an indispensable technique for the development of future organic devices.

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![Schematic diagram of vacuum deposition unit.](image)

**Figure A.2:** Schematic diagram of vacuum deposition unit.
Appendix D

Metal Phthalocyanines ($C_{32}H_{18}MN_8$)

Metal phthalocyanines (MePc) are macrocyclic metal complexes with 18 $\pi$-electrons in the microcyclic ring and mostly used as dyes. MePc molecules consist of a four fold $\pi$-conjugating macrocyclic ring in which four iso-indoline groups are bound by aza-nitrogens. A huge number of metal-phthalocyanines (Me-Pcs) can be formed with same molecular structure (as shown in Fig.3), which provides versatile and flexible chemical systems (central ion and substituents). Phthalocyanines are widely used as photoconductors in printer and photocopier industry because of its exceptional thermal and chemical stability. There is no noticeable degradation up to 400-500°C in air, 900°C in vacuum and no effect to strong acids/bases. The easily sublimated nature of MePcs make it possible to get these materials in high purity ($10^{13} - 10^{16}$ traps/cm$^3$), which allows the easy fabrication of high-quality thin films. Different types of MePc and its’ cousin porphine have attracted much interest because of their high chemical stability, various synthetic modifications and unique optical properties[30]. It has been realized recently that MePc is promising material for OLED and thin film transistor and MePc does not show degradation with time, which is commonly observed in other organic semiconductors.

![Figure A.3: Molecular structure of (a) CuPc and (b) Zn-Pc.](image_url)
Appendix E

tris, 8-hydroxyquinoline Aluminum($C_{27}H_{18}N_3O_3Al_1$)

An individual Alq3 molecule consists of a central Aluminum atom coordinated by three quinolate ligands, each of which binds to the metal site via oxygen and nitrogen donors, therefore giving a pseudo-octahedral environment for the Aluminum. Geometrically Alq3 can have two isomers, the meridianal and facial forms having $C_1$ and $C_3$ symmetries, respectively. Both experimental[130] and theoretical[131, 132] studies indicate that sl mer-Alq3 is the dominant form. It has been observed that the mer-Alq3 is of lower formation energy[132] than fac-Alq3 and mostly observed in thermally grown thin film. Both forms are shown in the Fig.A.4. The dipole moments of both the isomers are large. In the meridian isomer, the dipole is oriented towards the oxygen atom, which has a nitrogen trans to it (i.e., the oxygen pointing upwards and perpendicular to the paper). In the facial isomer, it points to the center of the triangular face defined by the three oxygen coming out of the plane. The ground state electronic properties were studied[133, 134] and the solid state properties were discussed with optimization. In meridian isomer, all the three Oxygen atoms are almost in one plane and the three Nitrogen atoms are on another perpendicular plane. All three quinoline radicals are basically perpendicular to each other.

Figure A.4: The (i) meridian and (ii) facial forms of Alq3.
Appendix F

Excitons in Organic Molecules

Exciton is a neutral particle moving through the crystal carrying the excitation energy. Excitonic effects are well known in many solid state systems, including ionic crystals, inorganic semiconductors and molecular organic crystals\[50, 135, 136\]. An exciton can be considered as a bound electron hole pair. There are three types of excitons.

A. Frenkle exciton: In this case, electron-hole (e-h) pair is located on one molecular unit. The neutral state can be considered as a tight e-h pair held together by a strong Coulombic interaction. The Frenkle exciton is highly localized (as shown in Fig.A.5b) and is often found in molecular solids where the molecules are not densely packed. Organic materials usually have low dielectric constant, hence the corresponding Coulombic interactions are large and Frenkle excitation model is suitable for the optical studies.

B. Mott-Wannier exciton: In this case, e-h pair extends over many molecular units (as shown in Fig.A.5a) and exciton radius is considerably larger than the intermolecular spacing. These excitons are observed in materials with low electron/hole effective mass ($m^*$) and large dielectric constant resulting small coulombic interaction (mostly observed in group IV and III-V inorganic semiconductors). The intermediate case, where the exciton extends over a few adjacent molecular units are called charge-transfer excitons.

Figure A.5: Schematic representation of (a) Mott-Wannier excitons (b) Frankle and.
Appendix G

Tunneling Current in Various Structures with Ultrathin Insulating Layer

Electric transport through the thin insulating film in devices will be dominated by quantum mechanical tunneling. Fowler-Nordheim mechanism is most commonly used method to explain the experimental J-V characteristics dominated by tunneling current. The expression for Fowler-Nordheim tunneling (FNT) current density is given by

\[ J_{\text{FNT}} = A F^2 \exp \left( -\frac{B}{F} \right) \]  

where,

\[ A = \frac{e^3}{8\pi \hbar \phi_B} \text{ and } B = -4\sqrt{2m^*(e\phi_B)^{3/2}/e\hbar} \],

\( F \) is the applied electric field, \( \phi_B \) is the barrier height formed at the junction, \( h \) is Plank's constant, \( e \) is the electronic charge and \( m^* \) is the carrier effective mass.

It has been found that FNT mechanism fails to fit the experimental data over wide range of electric field. This model ignores the image charge effects and is insensitive to temperature. The J-V characteristics of metal-insulator-semiconductor (MIS), metal-insulator-metal (MIM), metal-semiconductor-metal (MSM) and semiconductor-insulator-semiconductor (SIS) structures are determined numerically by solving the time dependent Schrodinger equation, which can explain the experimental data over wide range of bias. Also we have applied this to analyze the tunneling behavior of electrons and holes in MSM structures.

FNT expression (Eq.A.10) has calculated by considering the W.K.B approximation, which can explain experimental data only in the intermediate and cannot explain in the low and high electric fields. Here, we have solved time dependent Schrodinger equation numerically for a quantum mechanical tunneling through a square potential barrier. The shape of the potential will change with the applied electric field. This gives the exact shape of the J-V curve of different structures with thin insulating layer[138, 139, 140], when the insulating layer is very thin(\( \sim \) nm). This model can be applied to all types of heterostuctures, such as MIM, MIS, and SIS, if we know the shape of the potential formed at the junction.
Description of the Model for Tunneling Current Density

Figure A.6: Schematic flat energy band diagram for an ultrathin insulating film sandwiched between semiconductor and a metallic contact for zero bias (thin line) and biased with an applied voltage \( V_a \) (thick line).

A Gaussian wave packet localized in the semiconductor region, with an initial wave function of the form

\[
\psi(x, t = 0) = A\exp(ikx) \exp\left(-\frac{(x - x_c)^2}{2\sigma^2}\right)
\]

where \( A \) is the normalization constant, \( x_c \) is center of the wave packet, \( \sigma \) is the width of the wave packet and \( k \) is the packet's central wave number. The evolution of a one dimensional wave function \( \psi(x,t) \) is determined by solving time-dependent Schrodinger equation

\[
H\psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t),
\]

where \( H \) is the Hamiltonian operator associated with the system. Here \( H \) is taken to be of the Ben-Danial and Duke form\[141\], which is given by

\[
H = -\frac{\hbar^2}{2} \frac{\partial}{\partial x} \left[ \frac{1}{m^*} \frac{\partial}{\partial x} \right] + v(x)
\]
In operator form the evolution of the wave function $\psi(x,t)$ can be expressed as

$$\psi(x,t) = e^{-iHt/\hbar}\psi(x,0), \quad (A.14)$$

where $e^{-iHt/\hbar}$ is the time-development operator. The Ben-Danial and Duke Hamiltonian\[142\] is converted first to a difference equation as

$$H \psi_j = \frac{\hbar^2}{\epsilon^2} \left[ \frac{\psi_{j+1}}{m_{j+1}^* + m_j^*} + \frac{\psi_{j-1}}{m_{j-1}^* + m_j^*} - \frac{\psi_j}{m_{j+1}^* + m_j^* - m_{j-1}^* + m_j^*} \right] + V_j \quad (A.15)$$

where $\epsilon$ and $j$ are the space interval and space index, respectively. From Eq.A.13, we have

$$\psi_j^{n+1} = e^{-i\delta H / \hbar} \psi_j^n \quad (A.16)$$

where $\delta$ and $n$ are the time interval and time index, respectively. An approximation to preserve the normalization of the wave functions with time, $e^{-i\delta H / \hbar}$ can be converted into the Caley form $(1 - \frac{1}{2} i \delta H)/(1 + \frac{1}{2} i \delta H)$ to get

$$\psi_j^{n+1} = [(1 - \frac{1}{2} i \delta H)/(1 + \frac{1}{2} i \delta H)] \psi_j^n \quad (A.17)$$

Putting Eq.A.14 into Eq.A.16, it gives the finite-difference equation in the form

$$\frac{\psi_{j+1}^{n+1}}{m_{j+1}^* + m_j^*} + \left[ \frac{2\epsilon^2}{\hbar \delta} + \frac{\epsilon^2}{\hbar^2} V_j - \frac{1}{m_{j+1}^* + m_j^*} - \frac{1}{m_{j-1}^* + m_j^*} \right] \psi_j^{n+1} + \frac{\psi_{j-1}^{n+1}}{m_{j-1}^* + m_j^*}$$

$$+ \frac{\psi_j^{n+1}}{m_{j+1}^* + m_j^*} - \left[ \frac{2\epsilon^2}{\hbar \delta} + \frac{\epsilon^2}{\hbar^2} V_j + \frac{1}{m_{j+1}^* + m_j^*} + \frac{1}{m_{j-1}^* + m_j^*} \right] \psi_j^n + \frac{\psi_{j-1}^{n+1}}{m_{j-1}^* + m_j^*} = 0 \quad (A.18)$$

This finite difference equation is solved numerically\[141\] considering zero boundary conditions at 0.5 $\mu$m away from the junction\[143\] and taking $\epsilon = 0.3 \AA$ and $\delta = 5 fs$. The time integrated current density at a particular wave packet central energy $E$ at the probe position $x_0$ is calculated using the quantum mechanical current density expression

$$J_E = \frac{\hbar}{2m^* i} \left( \psi \frac{\partial \psi}{\partial x} - \psi^* \frac{\partial \psi^*}{\partial x} \right)|_{x=x_0} = Re \left( \psi \frac{\hbar}{im} \frac{\partial}{\partial x} \psi \right)|_{x=x_0} \quad (A.19)$$

Sum of all $J_E$ contributions of all electron wave packets in conduction band, which assumes the energy distribution

$$n(E) = \frac{b \sqrt{E}}{[1 + \exp((E - E_F)/k_b T)]} \quad (A.20)$$

will give the total current density. Here $E_F$ is the Fermi energy.
Observation of Tunneling Current in MIM and MIS Structures.

In the low electric field region \((F < F_c)\), the applied voltage is not sufficient to change the effective width of the barrier, hence the tunneling current is very small and almost linear. In the intermediate electric field region (near \(F_c\)), the current changes by several orders of magnitude over a relative small field range. Here the electric field is large enough to change the barrier width considerably and if the electric field increases, the effective width of the potential barrier formed at the junction decreases and tunneling current increases exponentially. In the high electric field region, tunneling current changes slowly with field and reaches a saturation current \(J_s\). Here the effective width is so small that all the electrons coming from the left region cross the barrier and can enter to the right side.

It is clear from the Fig.A.7 that for larger barrier, increase in \(\phi_B\) produces larger switching electric field \(F_c\) to influence on the effective width seen by tunneling electrons. These dependencies of tunneling current on applied electric field are in agreement with the experimental result [138, 139, 140] of the MIS structures taking \(Al/Ta_2O_5/si\), where \(Ta_2O_5\) is of 75nm thick. Time dependent Schrodinger equation can be used for simulation of future devices having tunneling as a dominant current transport process.

Figure A.7: Current-electric field characteristics of (a) MIS structure with 50nm insulator layer and (b) MIM structure with 150nm insulator layer for different barrier heights.
Appendix H

Commonly Observed Conduction Mechanisms in Crystalline Insulators

When a single carrier is injected into a semiconductor from a reservoir contact (i.e., the contact is able to supply sufficient current required by the bulk), the transport can be described by Ohmic, space charge limited conduction (SCLC) [144], and trap charge limited conduction (TCLC), which have been proposed as the charge carrier transport processes in semiconducting/insulating materials [23, 24, 25].

I. Ohmic Conduction

When there is no contact resistance at the electrode junction and in the absence of any localization in the material then, the current density $J$ is directly proportional to the applied field, satisfying the Ohm’s law as:

$$J = e\sigma F = e\mu p F$$  \hspace{1cm} (A.21)

where $\sigma$ is the conductivity, $\mu$ is the mobility and $p$ is the hole density. The applied electric field $F = V/L$, where $V$ is the applied voltage and $L$ is the distance between the two electrodes.

The hole density for moderate temperature can be expressed as,

$$p = \frac{N_V N_A e^{-E_T / k_B T}}{N_T}$$  \hspace{1cm} (A.22)

where $N_v$ is the effective density of states, $N_a$ is the acceptor density, $N_T$ is the trap concentration and $E_T$ is the trap energy. Hence the Ohmic current density expression is

$$J = e\mu \frac{N_V N_A e^{-E_T / k_B T} V}{L}$$  \hspace{1cm} (A.23)

II. Space charge Limited Conduction

In case of semiconductor/insulator with, when a single carrier is injected into a semiconductor from a contact, which is able to supply sufficient current required by the bulk, the total current will be limited by the build up of the space charges within the semiconductor. The formation of a strong space charge instability is dependent on the condition that the
necessary amount space charge can be build-up with in the transient time of the carriers. Space charges include the mobile ions and the ionized traps inside the insulator.

The space charge limited current has been observed in the low mobility thin film devices subject to the condition that at least one contact should be ohmic. Here at the ohmic contact the carriers will be injected from metal to semiconductor. As the mobility is very low, space charge is formed at the interface on the semiconductor side. After applying electric field the space charges will increase and the coulombic repulsion will restrict the further injection of carriers, hence limits the current flow. This is the space charge limited current. The SCLC is the maximum unipolar current a sample can sustain at a given electric field unless the exit contact is able to inject opposite charge carriers sufficient to compensate the internal space charge.

**Conditions to observe SCLC**

(i) The insulators must be relatively free from traps.

(ii) A necessary condition for SCL conduction is that one of the contacts should supply more charge carriers per unit time then can be transported trough the organic dielectric[20, 23, 50, 145]. A contact that behaves in this way is called an Ohmic contact in the sense of a charge carrier reservoir which can supply an excess of carriers ready to enter into the insulator as needed. At ohmic contact the electric field vanishes owing to screening by the space charge associated with unipolar current flow. This requires an injection barrier small enough to guarantee efficient injection without the assistance of an external electric field.

To get a good Ohmic contact, for a n-type semiconductor, a metal with work function less than the electron affinity of the semiconductor has to be chosen, so that electrons from the metal side will flow to the semiconductor in order to align the Fermi level of both the metal and semiconductor. The electron density at the interface will be more in the semiconductor side and as a result, band bending will take place at thermal equilibrium. Negative space charge will be formed in the semiconductor due to ionized dopants. So the metal in this case makes an ohmic contact with the semiconductor. If the work function of the metal be greater than the electron affinity of the semiconductor, then electron can not flow from metal to semiconductor easily due to the formation of a barrier(equal to the difference between the electron affinity of the semiconductor and the work function of the metal) for electron flow at the interface. This gives the formation of Schottky contact. Similarly to make ohmic to hole injection, the metal work function should be greater than the ionization potential of the semiconductor.
A. In thin perfect trap free insulating crystals with negligible free carrier concentrations in thermal equilibrium, all injected electrons remains free, i.e., in the conduction band and all contribute to the space charge. Neglecting the diffusion current, the current density is calculated by solving the Poisson’s equation together with

\[ J = \rho \mu F \]  \hspace{1cm} (A.24)

Where \( \rho \) is charge density, \( \mu \) is the mobility and \( E \) is the applied electric field.

Poisson’s equation is

\[ \frac{\partial F}{\partial x} = \frac{\rho}{\varepsilon_0} \]  \hspace{1cm} (A.25)

Solving these two equations for electric field considering the boundary condition of zero electric field at ohmic contact at \( x=0 \), and then integrating over the whole length we can get the expression for the applied voltage. The corresponding current expression is

\[ J = \frac{9\varepsilon_0 \mu V^2}{8L^3} \]  \hspace{1cm} (A.26)

This is the Child’s law[144], which is purely space charge limited with no traps.

B. SCLC with traps distributed in the band gap

The trapping levels which are present in the forbidden gap of an insulator or semiconductor, consist of many localized states due to imperfections in a crystal caused by structural defects and impurities. Discrete trapping levels due to the chemical impurities introduced into the lattice during growth which do not themselves trap the carriers. The polarization energy due to a charge carrier localized near an imperfection site in the crystal is different from that in a perfect lattice thus resulting in trapping of the carriers in the imperfection site. The formation, depth and concentration of the traps are directly dependent on the conditions under which the crystals are grown and the structure of the crystal. Structural imperfections are present in crystals in the form of fissures, crystalline boundaries, grain boundaries, dislocations and point defects. Any structural defects which perturb the periodic nature of the lattice will perturb the nature of charge carriers and hence the electric conductivity. These defects act as traps and include dislocations and planar defects (low angle lineage and grain boundaries). Experimentally, the point defects and concentration of dislocations can be reduced through an annealing process for the study of other electronic properties of the device made out of the material. If some traps present in the semiconductor, then the space charges which limits the current flow is stored in the traps. The number of
free charge carriers under given conditions then depends on the position of the quasi-Fermi level.

When traps are shallow in nature then SCLC will be same as in the case of trap free insulators by inserting a factor in mobility

$$\mu = \mu_0 \theta$$  \hspace{1cm} (A.27)

where \(\theta = \left( \frac{N_C}{N_T} \right) e^{\frac{-E_T}{kT}}\)

Here \(N_T\) represents the density of trap states which are all assumed to have equal energies, \(N_C\) is the no. of carriers injected into conduction band per \(cm^3\) and \(E_T\) is the trap depth.

Traps distributed exponentially: Structural defects introduce relatively deep traps and recombination centers which have an exponential distribution of trapping levels in the forbidden gap. Here the SCLC theory with an exponential trap distribution proposes that the space charge which limits the conduction is stored in the traps. The number of free charge carriers under given condition then depends on the position of the quasi-Fermi level[137, 50]. In this situation, the corresponding one carrier dominated transport is given by

$$J \propto \frac{V^{m+1}}{L^{2m+1}}$$ \hspace{1cm} (A.28)

where \(m = T_0/T > 2\) is a constant and \(T_0\) is the characteristic temperature.
Appendix I

Photoluminescence Spectroscopy

Photoluminescence (PL) is the optical emission obtained by photon excitation (usually a laser) and is commonly observed in semiconductor materials. PL spectroscopy is a contactless, nondestructive method of probing the electronic structure of materials. Light is directed onto a sample, where it is absorbed and imparts excess energy into the material in a process called photo-excitation. One way this excess energy can be dissipated by the sample is through the emission of light, or luminescence. In the case of photo-excitation, this luminescence is called "photoluminescence." The intensity and spectral content of this photoluminescence is a direct characterization of various important material properties such as band gap determination, impurity levels and defect detection, recombination mechanisms involved, and material quality. Specifically, photo-excitation causes electrons within the material to move into permissible excited states. When these electrons return to their equilibrium states, the excess energy is released and may include the emission of light (a radiative process) or may not (a non-radiative process). The energy of the emitted light or photoluminescence is related to the difference in energy levels between the two electron states involved in the transition that is, between the excited state and the equilibrium state i.e. ground state. The quantity of the emitted light is related to the relative contribution of the radiative process.

Thin films of desired thicknesses were grown over glass substrates with Vacuum deposition technique (Appendix C). The photoluminescence (PL) spectra were collected in the wavelength region of 300-1000nm by exposing to excitation with wavelengths 325nm and 488nm from Kimmon HeCd and American Laser Corp. Ar-ion lasers, respectively. Filter was used to block any light shorter than 340nm in the way to collect the luminescence. The samples were mounted in optical closed air cooled 8200 CTI-Cryogenics closed-cycle He refrigerator with quartz windows. Experiments were studied for different temperatures varied from 10K to 320K using a Lakshore 321 auto tuning temperature controller. The PL signal was collected into a 0.46 meter Jobin-Yvon grating monochromator and detected either with a liquid nitrogen cooled Ge detector or Si detector. The signal was processed with lock-in-technique using EG&G 7260 dual channel digital signal processor based lock-in-amplifier. Data collection was automated using desktop computer and National Instrument GPIB interfacing card. The schematic diagram of the PL setup is shown in Fig.A.9.
Figure A.9: Schematic Diagram of the Photoluminescence Measurement Setup
Appendix J

Absorption Spectroscopy

Absorption spectroscopy specifically UV-Vis Spectrometry has found its way to be a valuable tool for the analysis of the optical transitions of various organic and inorganic compounds. Thin films of organic molecular materials were grown on a glass or quartz substrates using vacuum deposition technique (more details is given in Chapter-II). The absorption spectra of thin film organic layers were taken using a Shimadzu, UV-2401PC spectrophotometer, which has a single monochromator with a high performance blazed holographic grating in the aberration corrected Czerny-Turner mounting. A schematic diagram of UV2401-PC spectrophotometer is shown in Fig.A.10. The low stray light/wide dynamic range/small beam size combination makes this single monochromator system well suited to handle a variety of practical situations, from small sample volumes to highly absorbing samples. The spectra were collected for Metal phthalocyanine(MePc) and tris, 8-hydroxyquinoline Aluminum(Alq3) organic thin films, in the wavelength range of 190nm to 900nm. The resulting spectra were analyzed using the software provided by the system package.

Figure A.10: Black diagram of the electrical systems of UV-2401PC

127
Appendix K

Atomic Force Microscopy

Atomic Force Microscope (AFM) has been used to characterize the morphology of the thermally deposited organic layers of CuPc and Alq3 on glass and Silicon substrates using vacuum deposition technique. The AFM images were taken using non-contact mode of vibrating-cantilever of Thrmomicroscopes AutoProbe CP AFM system. Non-contact mode is well suited for the low moduli samples such as organic thin films because in this method the cantilever tip does not come into contact with the sample surface, which avoids any kind of morphological damage (or surface distortion) at the time of scanning the surface. Non-contact AFM imaging, uses a vibrating cantilever tip held 50 to 100 Å above the simple surface during a scan. It is vibrated at a constant frequency near its mechanical resonant frequency (typically 50 to 400kHz), with an amplitude of a few tens of angstroms. As the tip scanned above the surface, the cantilever vibration amplitude changes in response to force gradients that vary with the tip-to-sample spacing. Surface topography is obtained by monitoring these changes in vibration amplitude. The simplified of the non-contact AFM system is shown in Fig.A.11.

Figure A.11: AFM setup in non-contact mode of vibrating cantilever method.
Appendix L

Interfacing

1. GPIB (General Purpose Interfacing Board)

Hardware Specifications:

[a] National Instruments GPIB-PC II/IIA CARD:

(i) Maximum GPIB Transfer Rates: 400 KB/sec.
(ii) Power Requirement (from PC/XT/AT I/O channel): +5 VDC, 250 mA (Typical) to 490 mA (Maximum).

[b] National Instruments AT-GPIB/TNT CARD:

(i) Maximum GPIB Transfer Rates: 1.5 MB/sec.
(ii) Power Requirement (from PC/AT I/O channel): +5 VDC, 50 mA (Typical) to 120 mA (Maximum).

Software Description:
The NI-488.2 software for DOS includes a loadable DOS device driver, language interface libraries, and debugging and development utilities. The NI-488.2 software and GPIB hardware transform a general-purpose PC into a GPIB Talker/Listener/Controller that has complete communications and bus management capacity.

2. ADDA (Analog to Digital and Digital to Analog Converter):

Card Type: ALS-PC-27
Power Requirements: 5V, 1.5A (max); +/- 12V, 100mA (max).
A/D CONVERTOR

* 16 bit A/D converter with conversion speed of 10 microseconds.
* Selectable unipolar/bipolar analog input (0 to +10V, +/-5V, +/--10V, 0 to +5V).

D/A CONVERTOR

* 12 bit programmable D/A converters.
* Selectable unipolar/bipolar operation ( +/-10v, 0 to 10v, 0 to +5v output range).

3. Programming Language: C

4. Data Acquisition Software Developed and Used:

* Current - Voltage characteristics.
* Capacitance - Voltage characteristics.
* Deep Level Transient Spectroscopy (DLTS).
* Admittance Spectroscopy.
* Photoluminescence Spectroscopy (PL).
* Photoconductivity Measurements.
* Thermally Stimulated Current Spectroscopy (TSC).