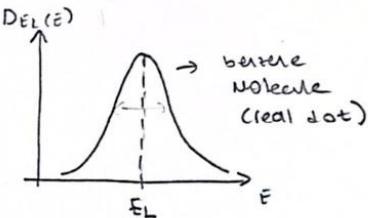
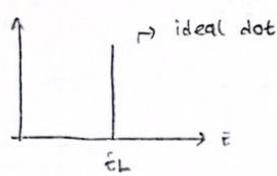


MICRO-435 HW8

Question 1

Explain Landauer Equation using as an example the case of the Benzene molecule

In a real molecule, the energy level E_L is not discrete.



$$D_{EL}(E) = \frac{\gamma/2\pi}{(E-E_L)^2 + \left(\frac{\gamma}{2}\right)^2}$$

$$T(E) = 2\pi \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} D_{EL}(E)$$

\downarrow
Transmission Spectrum

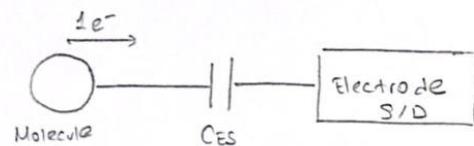
$$I_{DS} = \frac{q}{n} \int T(E) [f(E, E_{FS}) - f(E, E_{FD})] dE$$

Landauer Equation

Question 2

Explain Charging Effect in the case of the Benzene molecule with discrete levels

Charging Effect



* Electron injection shifts the energy

$$U_{\text{charging effect}} = -q \Delta V$$

$$= -q \left(\frac{-q}{C_{ES}} \right) = \frac{q^2}{C_{ES}}$$

$$\underbrace{\Delta Q}_{\pm q} = C_{ES} \cdot \Delta V$$

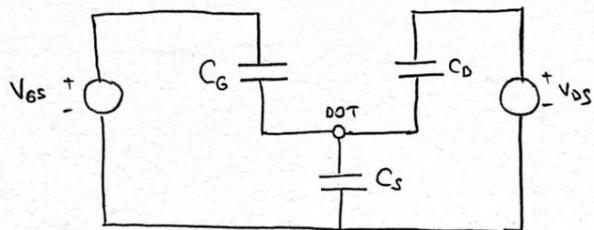
$\pm q$

$$-q = C_{ES} \Delta V \Rightarrow \Delta V = -\frac{q}{C_{ES}}$$

Question 3

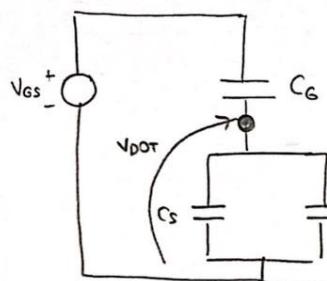
Discuss the effect of a gate voltage

Gating Effect

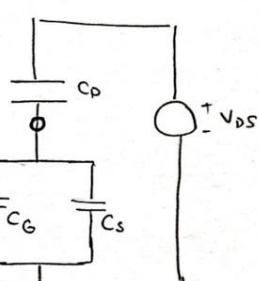


Using Superposition:

@ $V_{GS} = 0$



@ $V_{GS} = 0$



If $V_{GS} > 0$

$V_{DS} < 0$ \downarrow towards lower energies

If $V_{GS} < 0$

$V_{DS} > 0$ \uparrow toward higher energies

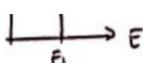
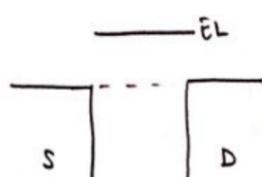
$$V_{GS} = -q \frac{V_{DDT}}{\epsilon_s} = -q V_{GS} \cdot \frac{C_G}{C_G + C_S + C_D}$$

Question 4

Consider the approximation of the MT model based on discrete levels, without charging effect, and without considering gating. In case of one single discrete level EL in the DOT calculate N and IDS (approximate) in case

- a) $V_{DS} = 0V$ and EL is bigger than both the energies of Source and Drain;

a)



$$I_{DS} = \frac{q}{h} \frac{2\gamma_1\gamma_2}{(\gamma_1+\gamma_2)} \left[f(EL, \bar{E}_{FS}) - f(EL, \bar{E}_{FD}) \right]$$

$I_{DS} = 0$

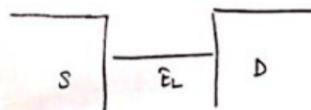
$$N = \frac{2}{\gamma_1 + \gamma_2} \left[\gamma_1 f(EL, \bar{E}_{FS}) + \gamma_2 f(EL, \bar{E}_{FD}) \right] = \frac{2}{\gamma_1 + \gamma_2} (\gamma_1 \gamma_2) \frac{1}{1 + e^{(EL - \bar{E}_{FS, D})/kT}}$$

$$N = \frac{2}{1 + e^{\frac{(EL - \bar{E}_{FS, D})}{kT}}}$$

N can be approximated to 0.

- b) $VDS = 0V$ and EL is smaller than both the energies of Source and Drain;

b)



$$I_{DS} = 0$$

$$N = \frac{2}{\tau_1 + \tau_2} (\tau_1 + \tau_2) f(\tilde{\epsilon}_L, \tilde{\epsilon}_{FS}) \underset{1}{\cancel{s}} \text{ (occupied states)}$$

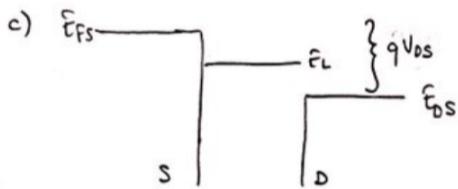
$$N = 2$$

$$\frac{1}{1 + e^{\frac{(\tilde{\epsilon}_L - \tilde{\epsilon}_{FS})/kT}{\cancel{1}}}} \approx 1$$

$$\frac{1}{e^{\frac{(\tilde{\epsilon}_{FS} - \tilde{\epsilon}_L)/kT}{\cancel{1}}}}$$

- c) $VDS > 0V$ and EL is between the energy level of the source and that of the drain

c)



$$\tilde{\epsilon}_{FD} = \tilde{\epsilon}_{FS} - qV_{DS}$$

$$\tilde{\epsilon}_L - \tilde{\epsilon}_{FS} = -\frac{qV_{DS}}{2}$$

$$\tilde{\epsilon}_L - \tilde{\epsilon}_{DS} = \frac{qV_{DS}}{2}$$

$$I_{DS} = \frac{q}{h} \frac{2\tau_1\tau_2}{\tau_1 + \tau_2} \left[f(\tilde{\epsilon}_L, \tilde{\epsilon}_{FS}) - f(\tilde{\epsilon}_L, \tilde{\epsilon}_{FD}) \right] = \frac{q}{h} \frac{2\tau_1\tau_2}{\tau_1 + \tau_2} \left[\frac{1}{1 + e^{-qV_{DS}/kT}} - \frac{1}{1 + e^{qV_{DS}/kT}} \right]$$

$$I_{DS} = \frac{q}{h} \frac{2\tau_1\tau_2}{\tau_1 + \tau_2} \left[\underbrace{\frac{e^{-qV_{DS}/kT}}{1 + e^{-qV_{DS}/kT}}}_{1} \right]$$

Assume $e^{qV_{DS}/kT} \gg 1$

$$I_{DS} = \frac{q}{h} \frac{2\tau_1\tau_2}{\tau_1 + \tau_2}$$

$$N = \frac{2}{\tau_1 + \tau_2} \left[\tau_1 f(\tilde{\epsilon}_L, \tilde{\epsilon}_{FS}) + \tau_2 f(\tilde{\epsilon}_L, \tilde{\epsilon}_{FD}) \right]$$

$$\frac{1}{1 + e^{-qV_{DS}/kT}}$$

$$N = \frac{2}{\tau_1 + \tau_2} \cdot \tau_1$$

If coupling factors are same N can be approximated as 1.

Question 5

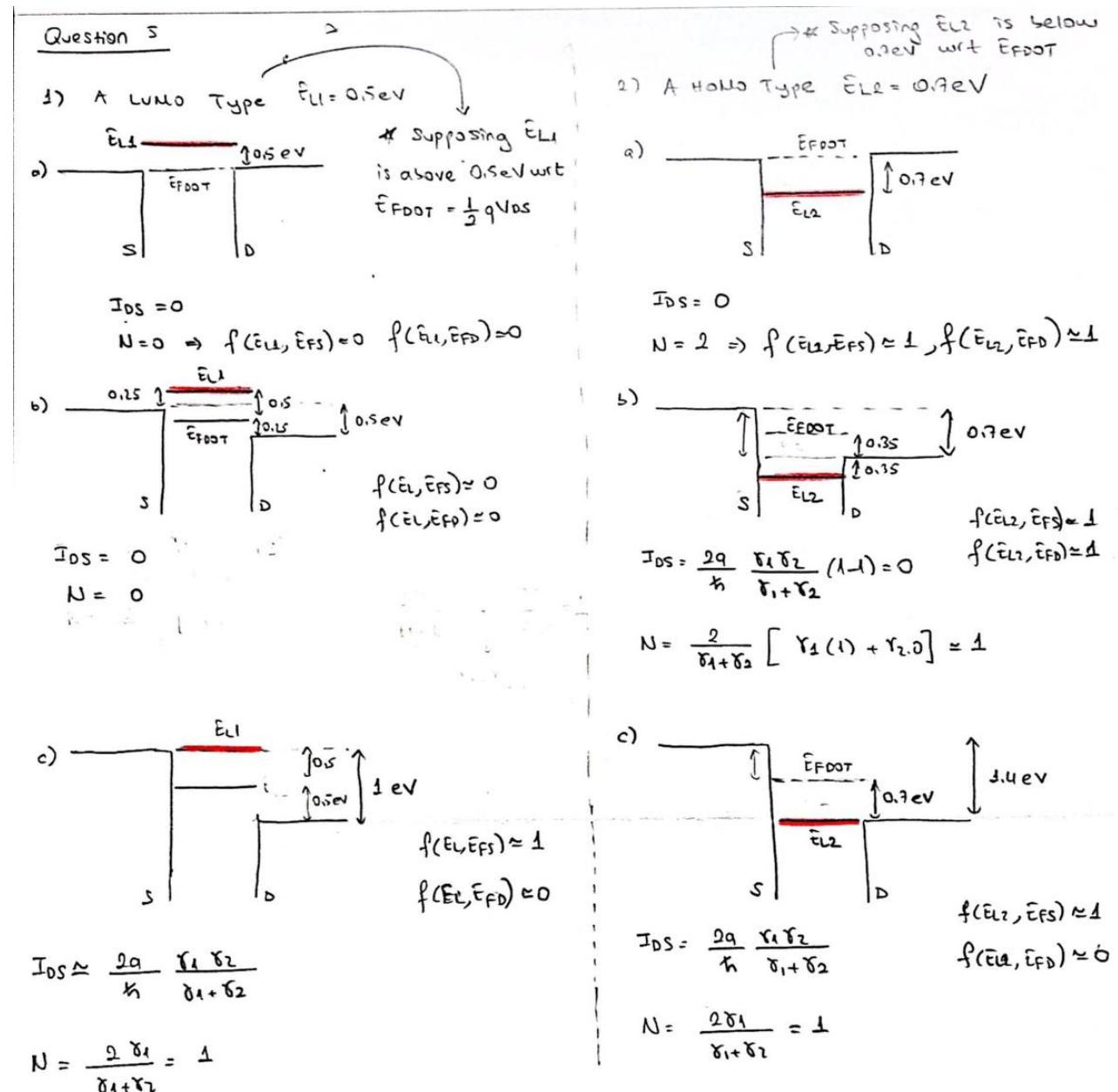
Consider the approximation of the MT model based on discrete levels, without charging effect, and without considering gating. In case of one single discrete level EL in the DOT calculate N and IDS (approximate) in the following two cases

1. A LUMO type molecule with $E_{L1} = 0.5\text{eV}$

- a) VDS = 0V
- b) VDS = 0.5V
- c) VDS = 1V

2. A HOMO type molecule with $E_{L2} = 0.7\text{eV}$

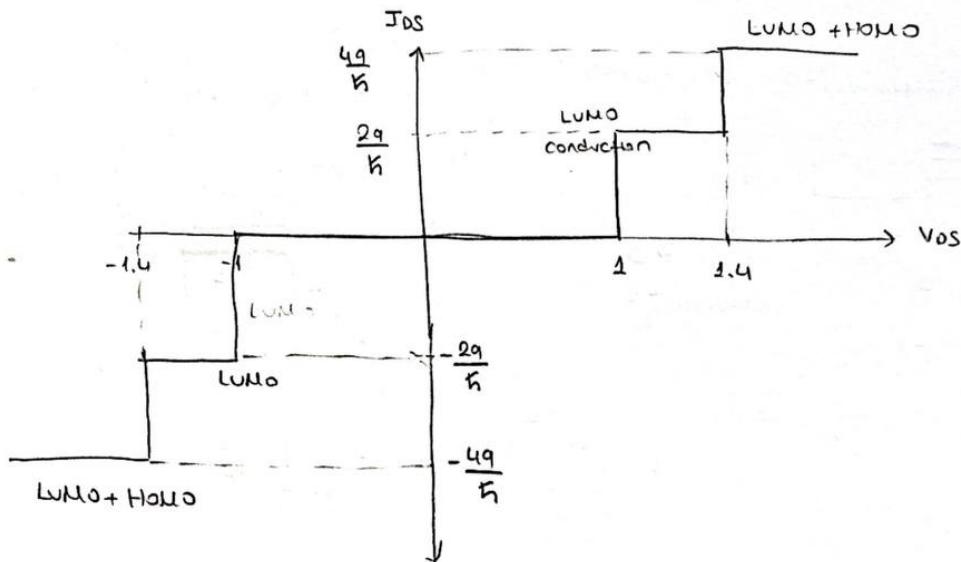
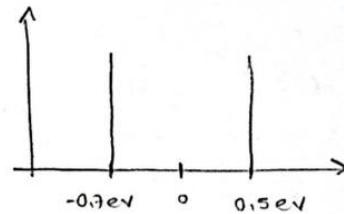
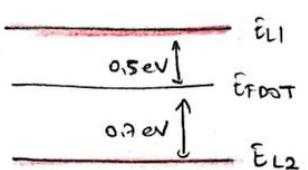
- a) VDS = 0V
- b) VDS = 0.7V
- c) VDS = 1.4V



Question 6

The Benzene molecule with the approximation of discrete level has as HOMO and LUMO the two values of the previous exercise EL1 and EL2. Sketch IDS and explain the applied concepts.

Question 6



Question 7

Consider a Molecular Transistor with a Source, a Drain, a Gate with the following values:

$EH = -5.5 \text{ V}$, $EL = -3.5 \text{ V}$, $E_{\text{system}} F = -5 \text{ eV}$, $\gamma_1 = 0.1 \text{ eV}$, $\gamma_2 = 0.1 \text{ eV}$, $C_s = CD = 0.5 \text{ aF}$, $CG = 1 \text{ aF}$

For each of the following approximations in the model:

Step A Discrete level, no charging effect

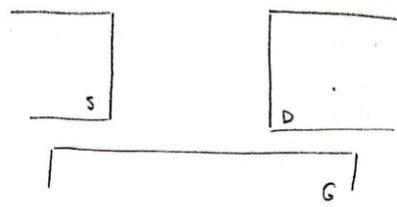
Step B Discrete level, with charging effect

Step C Broadening, no charging effect

Obtain and discuss the following quantities and characteristics

- $IDS(VG = 0, VDS=0)$
- $IDS(VG = 1, VDS=0)$
- $IDS(VG = -1, VDS=0)$
- $IDS(VG, VDS = 1)$

Question 7



$$E_H = -5.5 \text{ V}$$

$$E_L = -3.5 \text{ V}$$

$$E_{\text{systemf}} = -5 \text{ V}$$

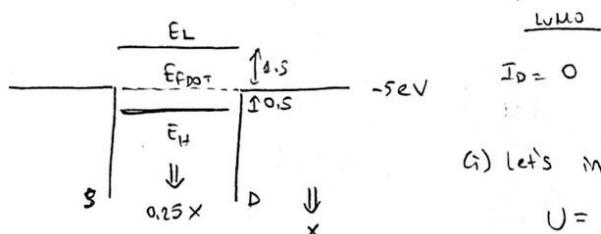
$$\gamma_1 = 0.1 \text{ eV}^{-1/2}$$

$$C_S = C_D = 0.5 \text{ aF}$$

$$C_G = 1 \text{ aF}$$

Step A Discrete level, NO C.E (charging effect)

i) I_{DS} ($V_{DS} = 0$, $V_G = 0$)



$$I_{DS} = \frac{2q}{h} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (1-1) = 0$$

ii) let's increase V_{DS}

$$U = U_{VDS} = -qV_{DS} \cdot \frac{C_D}{C_{ES}} = -q \cdot (V_{DS}) \frac{0.5}{2.4} = -0.75 V$$

when $E_H = E_{FD}$, conduction starts:

$$E_H - 0.25x = E_{FD} - x$$

↓
V_{DS} effect

$$-5.5 - 0.25x = -5 - x$$

$$1x - 0.25x = -5 + 5.5$$

$$0.75x = 0.5$$

$$x = \frac{1/2}{3/4} = \frac{1}{2} \cdot \frac{4}{3} = \frac{2}{3} = 0.68 \text{ V}$$

ii) Also when $E_L = E_{FS}$ conduction starts as well.

$$E_L - 0.25x = E_{FS} \quad (\text{reference} \rightarrow \text{stays constant})$$

$$-3.5 - 0.25x = -5$$

$$-0.25x = -5 + 3.5$$

$$-0.25x = -1.5$$

$$\boxed{x = 6 \text{ V}} \rightarrow \text{HOMO} + \text{LUMO}$$

iii) $V_{DS} < 0$

$U_{VDS} > 0$ shifts up the energy

$$\bullet E_L + 0.25x = E_{FD} + x$$

$$-3.5 + 0.25x = -5 + x$$

$$-3.5 + 5 = (1 - 0.25)x$$

$$+1.5 = 0.75x$$

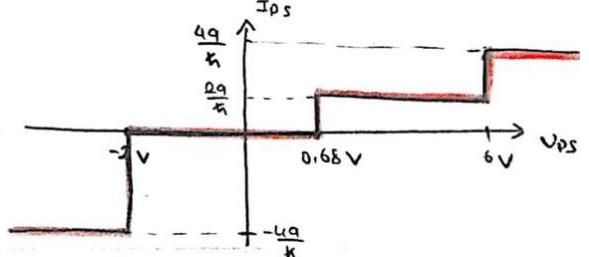
$$\boxed{x = +2 \text{ V}} \Rightarrow \boxed{-2 \text{ V}}$$

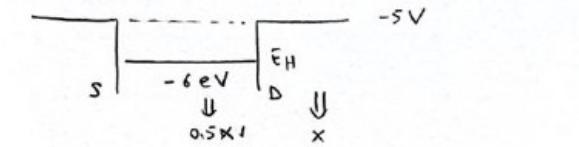
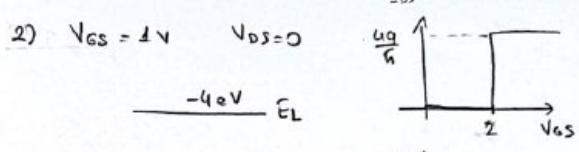
$$\bullet E_H + 0.25x = E_{FS}$$

$$-5.5 + 0.25x = -5$$

$$0.25x = -5 + 5.5$$

$$x = 2 \Rightarrow \boxed{x = -2 \text{ V}}$$





Gating Effect $V_G = -q \cdot \frac{C_G}{C_{GS}} (V_{GS}) = -0.5x \text{ eV}$

$I_{DS} = 0 \quad V_{GS} > 1$

$E_H = 0.5x = E_{FD} - x$

$-6 - 0.5x = -5 - x$

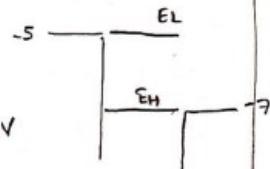
$(1 - 0.5)x = -5 + 6$

$0.5x = 1 \Rightarrow x = 2 \text{ V}$

$E_L - 0.5x = E_{FS}$

$-4 - 0.5x = -5$

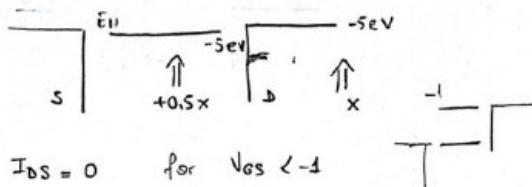
$-0.5x = -1 \Rightarrow x = 2 \text{ V}$



3) $V_{GS} = -1 \text{ V}$ $V_{DS} = 0$

$$U_G = -q \frac{C_G}{C_{GS}} (V_{GS}) = +q \frac{C_G}{C_{GS}} = +0.5x$$

$E_L = -3 \text{ eV}$



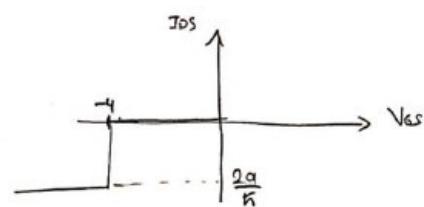
$I_{DS} = 0 \quad \text{for } V_{GS} < -1$

$E_L + 0.5x = E_{FD} - x$

$-3 + 0.5x = -5 + x$

$(40.5 - 1)x = -5 + 3$

$-0.5x = -2 \Rightarrow x = 4 \Rightarrow x = -4 \text{ V}$

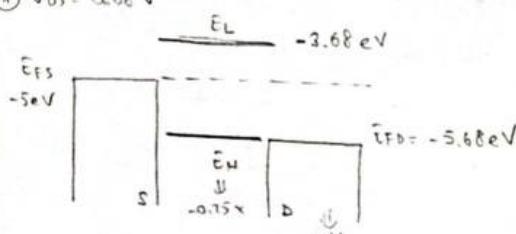


Step B Discrete levels with Coulomb effect

$$U_{TOT} = U_{VGS} + U_{VDS} + U_{CE} \xrightarrow{\frac{q^2}{C_{GS}} (N - N_s)}$$

let's focus the parts just after the injection

① $V_{DS} = 0.68 \text{ V}$



Homo level starts to conduct

$N = 2$

$V_{DS} > 0.68 \rightarrow N = ?$

$1 < N < 2$

$f(E_H, E_F) \approx 1, f(E_H, E_{FD}) \approx 0$

$N = \frac{2}{Y_1 + Y_2} (Y_1) = 1$

N reduces to 1

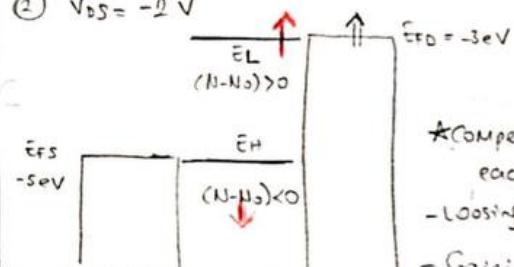
thus $|N - N_s| < 0$

$U_{CE} < 0$ shifted to lower energies

\Rightarrow Holes can escape from the bias window

\Rightarrow Current does not increase sharply as in the case w/o C.E.

② $V_{DS} = -2 \text{ V}$



*Compensate each other
-Loosing e's from LUMO
-Gaining e's from LUMO

③ $V_{DS} = 6V$

both HOMO and LUMO conduct.

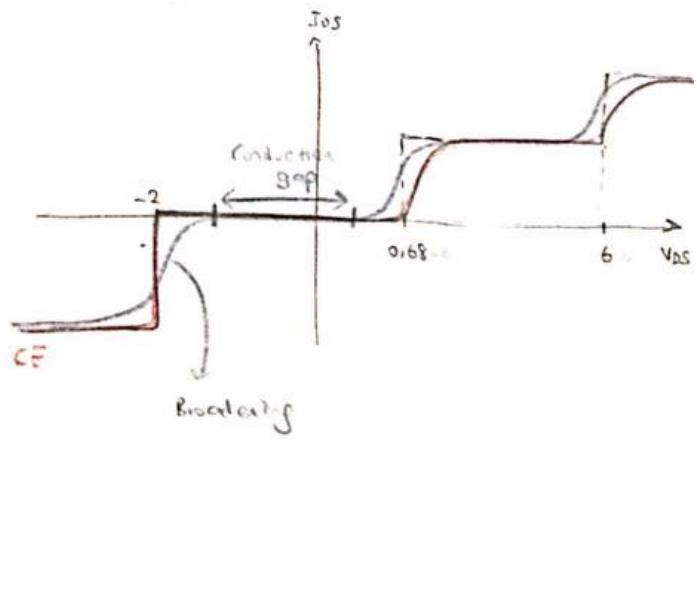
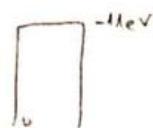
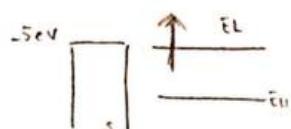
thus, new ϵ_s start to enter

$$|\epsilon_s - \epsilon_0| > 0$$

$\epsilon_c > 0 \rightarrow$ shifted to upper energies

* $V_{DS} \uparrow \epsilon_c$ enters more in BW

$|\epsilon_s - \epsilon_0| > 0$ effect reduces

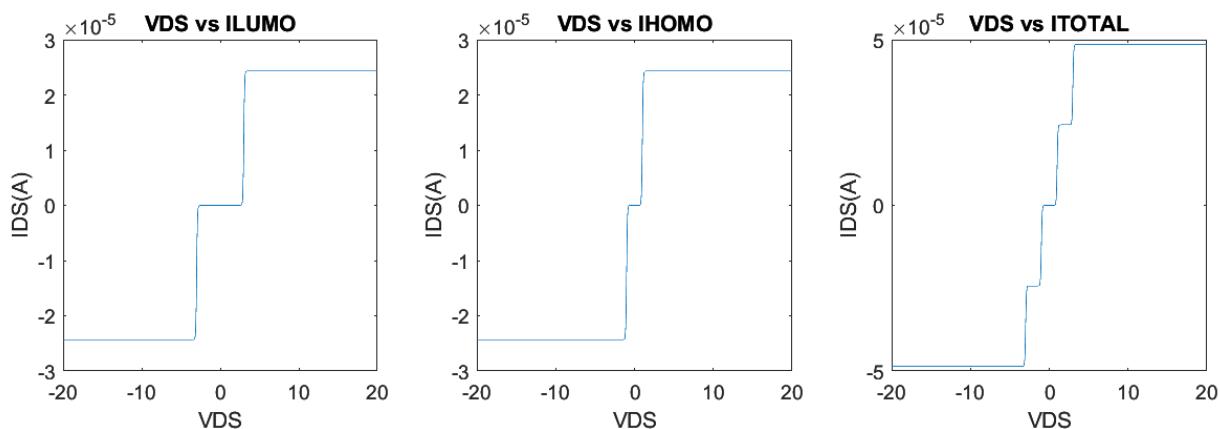


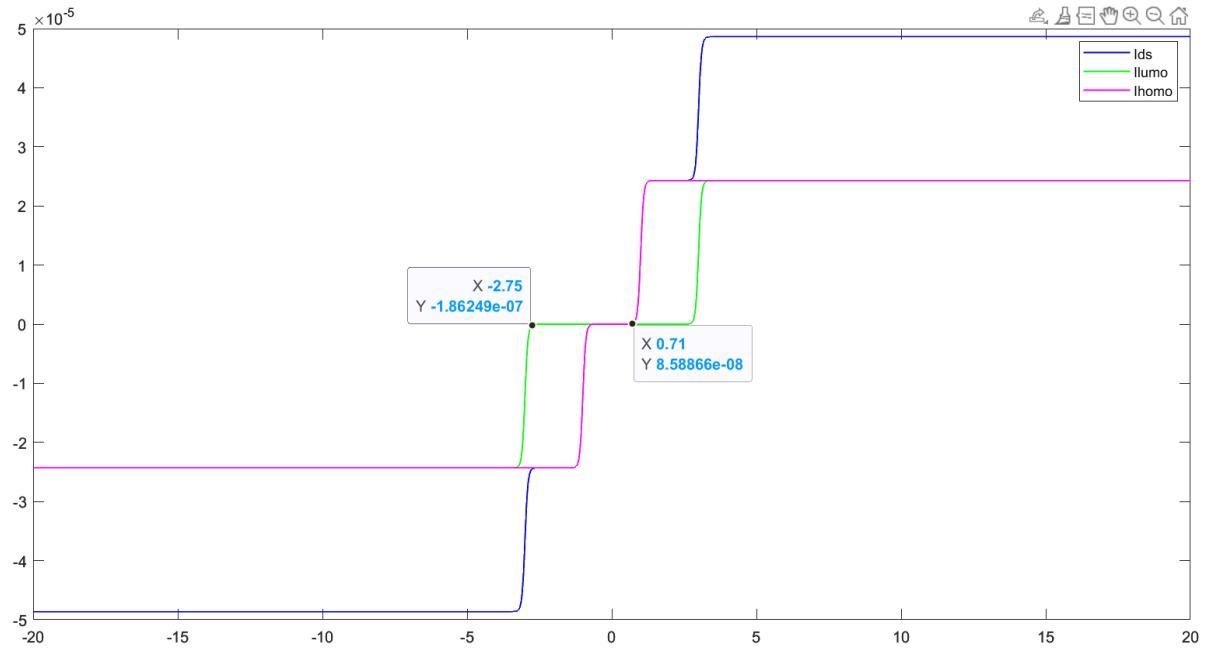
Question 8

Implement the equations for the IDS current in the DOT under the same hypotheses ad in Question 7 step A using MATLAB and

- Verify the values obtained in exercise 7, step A
- for the same case, calculate the values and plot the functions for $\gamma = 2\text{eV}$ and $\gamma = 0.3\text{eV}$, with the same value for the other indexes, and comment the results
- Calculate the same values as in exercise 7 step a for $T = 300\text{K}$ and $T = 400\text{K}$, plot the functions and comment the results

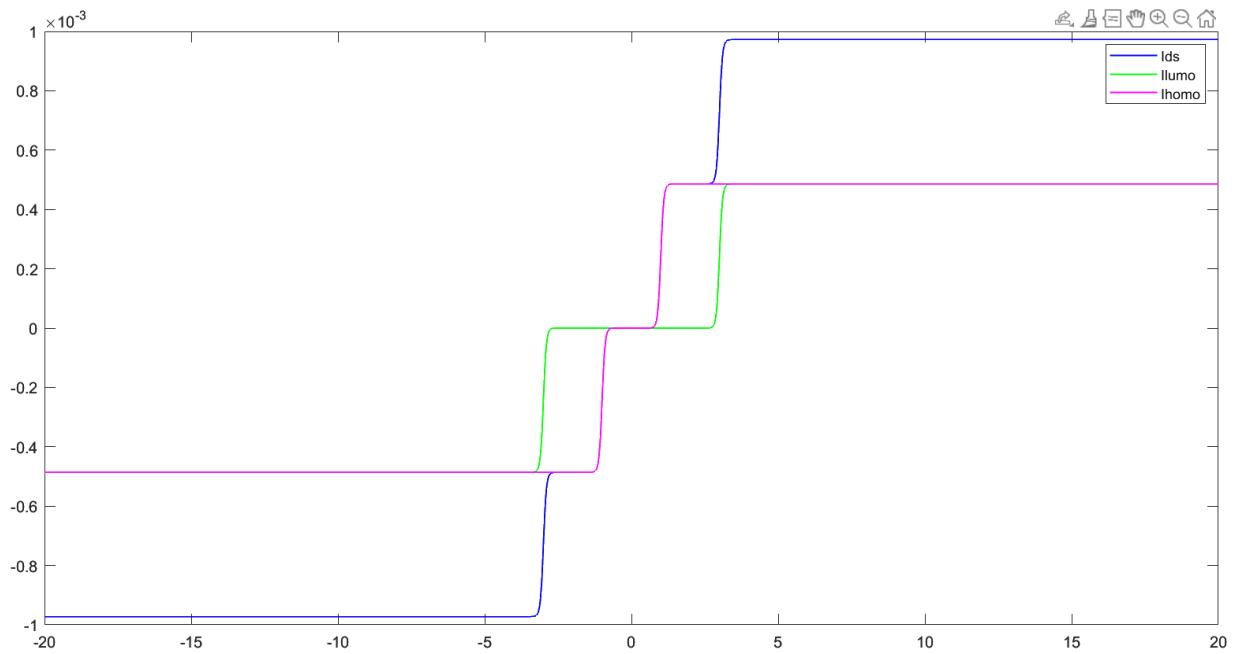
a)

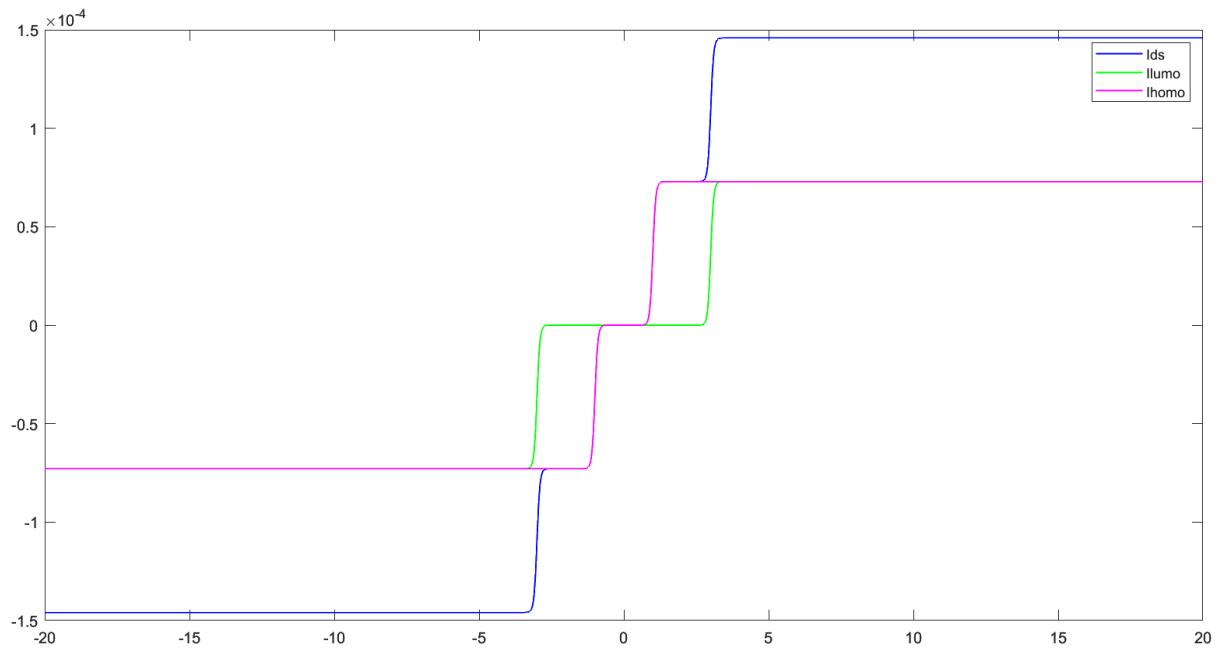




Results are similar except HOMO conduction starts at 6 V in calculations. In MATLAB conductances start at 0.71V and -2.75V.

b)

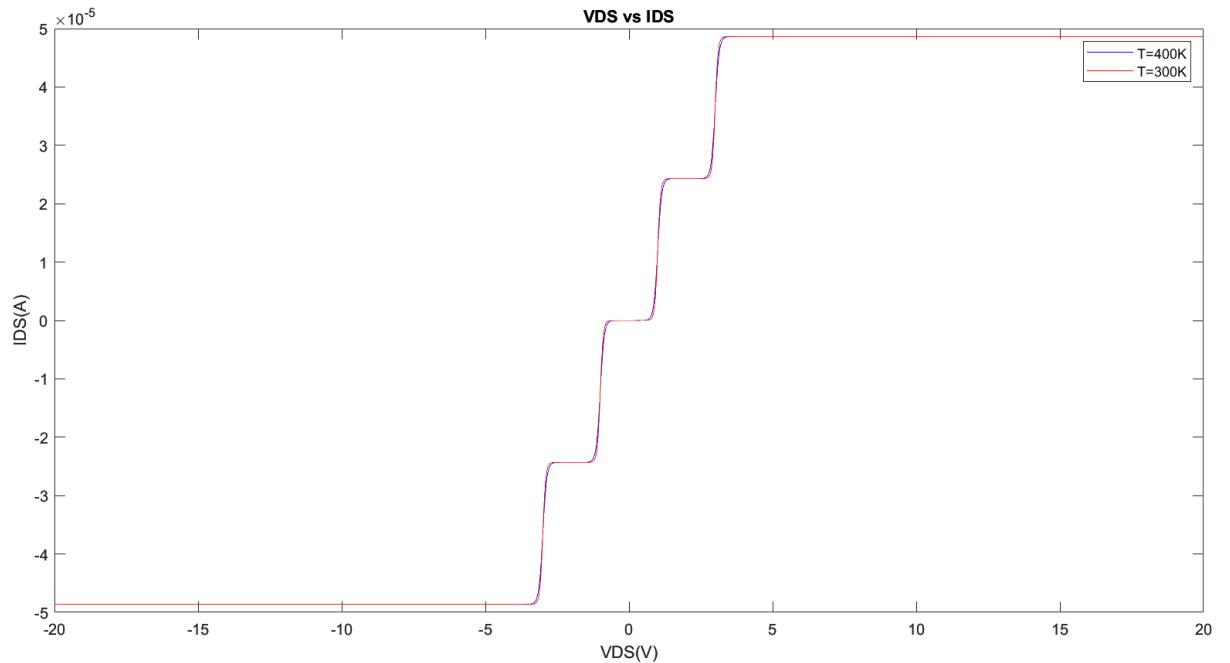




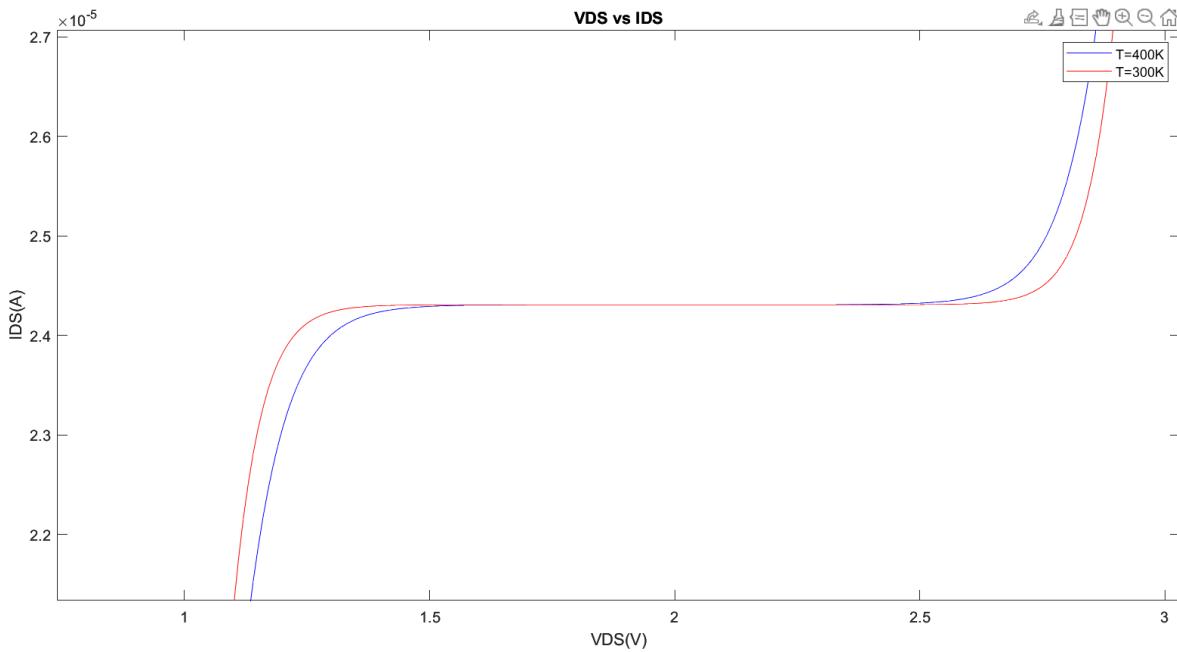
Gammas are 0.3 eV

As expected changing gama changes current proportionally as in the approximated formula.

c)



Results are quite similar to each other.



Conduction gap is smaller for T=400K.

Question 9

Estimates the equations for the IDS current in the DOT under the same hypotheses ad in Question 7 step B using matlab

$$\text{SCF} \left[\begin{array}{l} N = \frac{2}{\gamma_1 + \gamma_2} \int_{-\infty}^{\infty} D_{eL}(E-U) [\dots] dE \\ U_{CE} = U_0 (N - N_0) \\ U_0 = \frac{q^2}{C_{ES}} \end{array} \right]$$

For HOMO

$$N_{HOMO} = \frac{q}{\gamma_1 + \gamma_2} \int \delta(E - E_{HOMO} - U_{DOS}) [\gamma_1 f(E, E_{FS}) + \gamma_2 f(E, E_{FD})] dE$$

$$N_{HOMO} = \frac{2}{\gamma_1 + \gamma_2} \left[\gamma_1 f(\tilde{E}_{HOMO} + U_{DOS}, E_{FS}) + \gamma_2 f(\tilde{E}_{HOMO} + U_{DOS}, E_{FD}) \right]$$

$$U_{CE} = \frac{q^2}{C_{ES}} (N_{HOMO} - N_0)$$

$$IDS_{HOMO} = \frac{q}{h} \frac{2\gamma_1\gamma_2}{\gamma_1 + \gamma_2} \left[f(E^*, E_{FS}) - f(E^*, E_{FD}) \right]$$

For LUMO

$$N_{LUMO} = \frac{2}{\gamma_1 + \gamma_2} \left[\gamma_1 f(\tilde{E}^*, E_{FS}) + \gamma_2 f(\tilde{E}^*, E_{FD}) \right]$$

$$U_{CE} = \frac{q^2}{C_{ES}} (N_{LUMO} - N_0)$$

$$IDS_{LUMO} = \frac{q}{h} \frac{2\gamma_1\gamma_2}{\gamma_1 + \gamma_2} \left[f(\tilde{E}^*, E_{FS}) - f(\tilde{E}^*, E_{FD}) \right]$$

$$E^* = E_{LUMO} + U_{DOS}$$

$$\text{where } U_{DOS} = U_{VGS} + U_{VDS} + U_{CE}$$

$$-qV_{DS} \cdot \frac{C_D}{C_{ES}} \quad \frac{q^2}{C_{ES}} (N - N_0)$$

```

%MICRO-435 HW8 Question 8
%IDS-VDS curve for Quantum Dot

Elumo_init=-3.5; %LUMO=lowest unoccupied molecular orbit-not used
Ehomo_init=-5.5; %HOMO=highest occupied molecular orbit-not used
Esystem=-5; %Fermi energy of the source as reference
Coupling1=0.1; %Source coupling factor
Coupling2=0.1; %Drain coupling factor
Cs=0.5*1e-18; %attofarad=10^-18 farad, Source capacitor
Cd=0.5*1e-18; %drain capacitor
Cg=1e-18; %gate capacitor

q=1.6*1e-19; %coulomb
hbar=6.582*1e-16; %eV.s
kT=25.7*1e-3; %eV
kT_400=34.2*1e-3;

%Define Vds
VDS=-10:0.1:10;

%Array sizes
Uvds=zeros;
Uce_homo=zeros;
Uce_lumo=zeros;
Udot_lumo=zeros;
Udot_homo=zeros;

Fermi_EL_Efs=zeros;
Fermi_EL_Efd=zeros;
Fermi_EH_Efs=zeros;
Fermi_EH_Efd=zeros;

Nhomo=zeros;
Nlumo=zeros;

IDS_LUMO=zeros;
IDS_HOMO=zeros;
IDS=zeros;

%Efdot changes with changing VDS
Efdot=Esystem-0.5*VDS;

%Elumo and Ehomo changes with changing VDS since Efdot changes
Ehomo=Efdot-0.5;
Elumo=Efdot+1.5;

for i=1:0.1:length(VDS)

    %UDOT coming from Uvds
    Uvds(i)=-q*VDS(i)*Cd/(Cd+Cs+Cg);
    Uce_homo(i)=q^2*(Nhomo(i)-2)/(Cs+Cd+Cg);
    Uce_lumo(i)=q^2*(Nlumo(i)-2)/(Cs+Cd+Cg);
    Udot_lumo(i)=Uvds(i)+Uce_lumo(i);
    Udot_homo(i)=Uvds(i)+Uce_homo(i);

```

```

%-----
%Fermi Function for ELumo and EHomo
%EFdrain=EFsource-VDS
Fermi_EL_Efs(i)=1./(exp(((Elumo(i)+Udot_lumo(i))-Esystem)/kT)+1);
Fermi_EL_Efd(i)=1./(exp(((Elumo(i)+Udot_lumo(i))-(Esystem-VDS(i)))/kT)+1);

Fermi_EH_Efs(i)=1./(exp(((Ehomo(i)+Udot_homo(i))-Esystem)/kT)+1);
Fermi_EH_Efd(i)=1./(exp(((Ehomo(i)+Udot_homo(i))-(Esystem-VDS(i)))/kT)+1);

%-----
Nhomo(i)=2/(Coupling1+Coupling2)*(Coupling1*Fermi_EH_Efs(i)+Coupling2*Fermi_EH_Efd(i));
;

Nlumo(i)=2/(Coupling1+Coupling2)*(Coupling1*Fermi_EL_Efs(i)+Coupling2*Fermi_EL_Efd(i));
;

%current formula for LUMO and HOMO at T=300K

IDS_LUMO(i)=(q*2*Coupling1*Coupling2)*(Fermi_EL_Efs(i)-Fermi_EL_Efd(i))/(hbar*(Coupling1+Coupling2));
IDS_HOMO(i)=(q*2*Coupling1*Coupling2)*(Fermi_EH_Efs(i)-Fermi_EH_Efd(i))/(hbar*(Coupling1+Coupling2));
IDS(i)=IDS_LUMO(i)+IDS_HOMO(i);
end

figure
plot(VDS,IDS,'b','LineWidth',1);
hold on
plot(VDS,IDS_LUMO,'g','LineWidth',1);
plot(VDS,IDS_HOMO,'m','LineWidth',1);
legend('Ids','Ilumo', 'Ihomo');

```

Appendix

Question 8 MATLAB Code

```
%MICRO-435 HW8 Question 8
%IDS-VDS curve for Quantum Dot

Elumo_init=-3.5; %LUMO=lowest unoccupied molecular orbit-not used
Ehomo_init=-5.5; %HOMO=highest occupied molecular orbit-not used
Esystem=-5; %Fermi energy of the source as reference
Coupling1=0.1; %Source coupling factor
Coupling2=0.1; %Drain coupling factor
Cs=0.5*1e-18; %attofarad=10^-18 farad, Source capacitor
Cd=0.5*1e-18; %drain capacitor
Cg=1e-18; %gate capacitor

q=1.6*1e-19; %coulomb
hbar=6.582*1e-16; %eV.s
kT=25.7*1e-3; %eV
kT_400=34.2*1e-3;

%define a VDS vector
VDS=-20:0.01:20;

%Efdot changes with changing VDS
Efdot=Esystem-0.5*VDS;

%Elumo and Ehomo changes with changing VDS since Efdot changes
Ehomo=Efdot-0.5;
Elumo=Efdot+1.5;

%-----
%UDOT coming from Uvds
Uvds=-q*VDS*Cd/(Cd+Cs+Cg);
Udot=Uvds;
%-----

%Fermi Function for ELumo and EHomo
%EFdrain=EFsource-VDS
Fermi_EL_Efs=1./(exp(((Elumo+Udot)-Esystem)/kT)+1);
Fermi_EL_Efd=1./(exp(((Elumo+Udot)-(Esystem-VDS))/kT)+1);

Fermi_EH_Efs=1./(exp(((Ehomo+Udot)-Esystem)/kT)+1);
Fermi_EH_Efd=1./(exp(((Ehomo+Udot)-(Esystem-VDS))/kT)+1);

%Fermi Functions for T=400K
Fermi_EL_Efs_400=1./(exp((Elumo-Esystem)/kT_400)+1);
Fermi_EL_Efd_400=1./(exp((Elumo-(Esystem-VDS))/kT_400)+1);

Fermi_EH_Efs_400=1./(exp((Ehomo-Esystem)/kT_400)+1);
Fermi_EH_Efd_400=1./(exp((Ehomo-(Esystem-VDS))/kT_400)+1);

%current formula for LUMO and HOMO at T=300K
```

```

IDS_LUMO=(q*2*Coupling1*Coupling2)*(Fermi_EL_Efs-Fermi_EL_Efd)/(hbar*(Coupling1+Coupling2));
IDS_HOMO=(q*2*Coupling1*Coupling2)*(Fermi_EH_Efs-Fermi_EH_Efd)/(hbar*(Coupling1+Coupling2));
IDS=IDS_LUMO+IDS_HOMO;

%current formula for LUMO and HOMO at T=400K
IDS_LUMO_400=(q*2*Coupling1*Coupling2)*(Fermi_EL_Efs_400-Fermi_EL_Efd_400)/(hbar*(Coupling1+Coupling2));
IDS_HOMO_400=(q*2*Coupling1*Coupling2)*(Fermi_EH_Efs_400-Fermi_EH_Efd_400)/(hbar*(Coupling1+Coupling2));
IDS_400=IDS_LUMO_400+IDS_HOMO_400;

%Fermi Energy Plots
subplot(2,4,1);
plot(VDS,Fermi_EL_Efs);
xlabel('VDS');
title('VDS vs f(EL,EFS)');

subplot(2,4,2);
plot(VDS,Fermi_EL_Efd);
xlabel('VDS');
title('VDS vs f(EL,EFD)');

subplot(2,4,3);
plot(VDS,Fermi_EH_Efs);
xlabel('VDS');
title('VDS vs f(EH,EFS)');

subplot(2,4,4);
plot(VDS,Fermi_EH_Efd);
xlabel('VDS');
title('VDS vs f(EH,EFD)');

%IDS Curves
subplot(2,4,5)
plot(VDS,IDS_LUMO)
xlabel('VDS');
ylabel('IDS(A)')
title('VDS vs ILUMO');

subplot(2,4,6)
plot(VDS,IDS_HOMO)
xlabel('VDS');
ylabel('IDS(A)')
title('VDS vs IHOMO');

subplot(2,4,7)
plot(VDS,IDS)
xlabel('VDS');
ylabel('IDS(A)')
title('VDS vs ITOTAL');

%EFDOT

```

```

subplot(2,4,8)
plot(VDS,Efdot)
xlabel('VDS')
ylabel('Efdot(eV)')
title('VDS vs Efdot')

figure
plot(VDS,IDS,'b','LineWidth',1);
hold on
plot(VDS,IDS_LUMO,'g','LineWidth',1);
plot(VDS,IDS_HOMO,'m','LineWidth',1);

legend('Ids','Ilumo', 'Ihomo');

figure
plot(VDS,IDS_400,'b','LineWidth',0.5);
hold on

% plot(VDS,IDS_LUMO_400,'g','LineWidth',1);
% plot(VDS,IDS_HOMO_400,'m','LineWidth',1);

plot(VDS,IDS,'r','LineWidth',0.5);
legend('T=400K','T=300K');

xlabel('VDS(V)');
ylabel('IDS(A)');
title('VDS vs IDS');

```