MICRO-435

Homework W9 - Conduction in MT

Qualitative Questions

Question 1 Explain Landauer Equation using as example the case of the Benzene molecule

Question 2 Explain Charging Effect in the case of the Benzene molecule with discrete levels

Question 3 Discuss the effect of a gate voltage

Quantitative Questions

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 E_L in the DOT calculate N and I_{DS} (approximate) in case

- a) $V_{DS} = 0V$ and E_L is bigger than both the energies of Source and Drain;
- b) $V_{DS} = 0V$ and E_L is smaller than both the energies of Source and Drain;
- c) $V_{DS} > 0V$ and E_L is between the energy level of the source and that of the drain

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 E_L in the DOT calculate N and I_{DS} (approximate) in the following two cases

1. A LUMO type molecule with $E_{L1} = 0.5eV$
   - a) $V_{DS} = 0V$
   - b) $V_{DS} = 0.5V$
   - c) $V_{DS} = 1V$
2. A HOMO type molecule with $E_{L2} = 0.7eV$
   - a) $V_{DS} = 0V$
   - b) $V_{DS} = 0.7V$
   - c) $V_{DS} = 1.4V$

Question 6 The Benzene molecule with the approximation of discrete level has as HOMO and LUMO the two values of the previous exercise E_{L1} and E_{L2}. Sketch I_{DS} and explain the applied concepts.

Question 7 Consider a Molecular Transistor with a Source, a Drain, a Gate with the following values:

$$E_H = -5.5V, E_L = -3.5V, E_F^{system} = -5eV, \gamma_1 = 0.1eV, \gamma_2 = 0.1eV, C_s = C_D = 0.5aF, C_G = 1aF$$

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 (approximately) and discuss the following quantities and characteristics

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

ii) $I_{DS}(V_G = 1, V_{DS})$

iii) $I_{DS}(V_G = -1, V_{DS})$

iv) $I_{DS}(V_G, V_{DS} = 1)$

Question 8 Implement the equations for the I_{DS} current in the DOT under the same hypotheses ad in Question 7 step A using MATLAB and

a) Verify the values obtained in exercise 7, step A

b) for the same case, calculate the values and plot the functions for $\gamma = 2eV$ and $\gamma = 0.3eV$, with the same value for the other indexes, and comment the results

c) Calculate the same values as in exercise 7 step a for $T = 300K$ and $T = 400K$, plot the functions and comment the results

Question 9 Estimate the equations for the I_{DS} current in the DOT under the same hypotheses ad in Question 7 step B using MATLAB

Question 10 OPTIONAL: Estimate the equations for the I_{DS} current in the DOT under the same hypotheses and in Question 7 step C using MATLAB