

MICRO-435

Exercises W11: Circuits and Transport Numerical Simulation

Question 1 - hierarchical array circuits with MT

Refer to the array structure used in exercise 1 of W10. In figure 1 the concept of cascading is shown: when the maximum number of transistor in the same array is reached, it is convenient to cascade two arrays. Technological parameters must be taken into account as parasitic resistance and capacitance of interconnect and of cascaded stages. Until the technology is not mature a regeneration stage might be necessary between two cascaded arrays (not shown) based on MT buffers of on standard technology buffers.



Figure 1: Cascading of two arrays of MTs

The direction the is the one shown in figure 2 where several arrays are cascaded, external signals are delivered to the arrays, and where partially processed functions are passed through staggered arrays, each dedicated to the elaboration of a subfunction. In this context design a Full Adder and associate it to a single Array

- Design a Full Adder and associate it to a single Array
- Design a Ripple Carry Adder and associate it to a Matrix, describing how to place the stages of Full Adders and how to route the signals to connect them
- OPTIONAL: Design a simple Array Multiplier, first defining the single stages and then placing and routing them on a matrix.

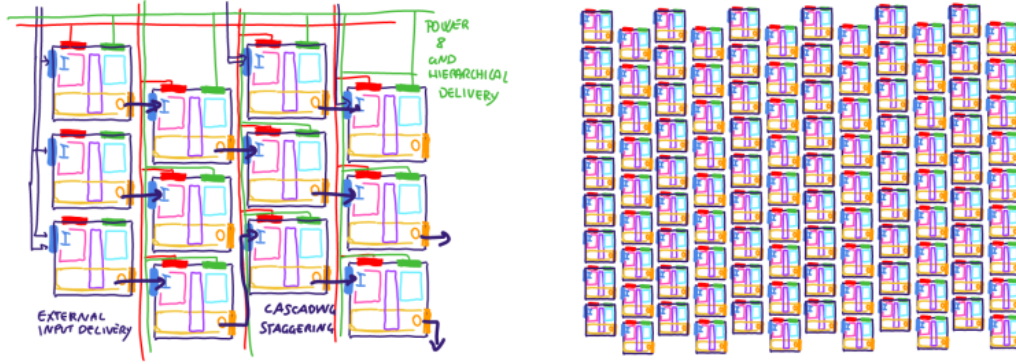


Figure 2: Left: a matrix of 9 arrays with signal and power delivery. Right: a generic extended matrix of MTarrays

Question 2: fabrication of MT and molecule selection

It is necessary to estimate for a CDBJ process the length L_{bridge} of the bridge wire to be fabricated. L_{bridge} must be chosen depending on the optimal number of rings N rings of a molecule derived by oligothiophene maximizing the I_o/I_{off} ratio of a MT.

- (a) Formulate the length L_{bridge} dependency on the number of rings N rings knowing that the average elastic strain ϵ for TiN is 0.0053 and that the crack in the bridge wire d_{wire} depends linearly on the crack in TiN w_{TiN} by a constant $k = 0.2$. Consider that a single ring length is approximately $l_{ring} = 2\text{nm}$
- (b) Analyze and sketch approximately the Transmission spectrum $T(E)$ and the Current $I(T(E))$ of the molecules with the increasing number of rings. Name the molecules M-1R, M-2R, and so on, the Transmission spectrum to be identified $T(E)_{1R}$, $T(E)_{2R}$ and so on, and the current I_{1R} , I_{2R} and so on. Explore up to a maximum of 5 rings. Consider a maximum BW of 5eV. Use the following simplified model:
 - in the simple case of 1 ring (M-1R) the HLG is 3.5eV, $E_F = 0\text{eV}$, HOMO and LUMO peaks are symmetrical w.r.t. E_F , and, considering broadening, the area A_{Lz90} associated to 90% of the Lorentian distribution corresponds approximately to a “Lorentian base” $LzB = 1\text{eV}$. Only the HOMO peaks and LUMO are included in the BW.
 - when the number of rings increases $HLG(N_{rings}) = 3.5 - \frac{(1-N_{rings})^2}{6}$
 - for each new ring introduced, a new peak (both in HOMO and LUMO sides) is introduced in the BW
 - when a new ring is considered the A_{Lz90} for each peak in the BW corresponds to a halved base LzB w.r.t. the case with the previous nr. of rings. For simplicity keep the same peak height as in the initial 1 ring situation.
 - when new peaks are added they are consecutive but not superposed (e.g. the HOMO and HOMO+1 peaks have two consecutive “Lorentian bases”)
- (c) Identify and discuss the optimum number of rings N_{rings} in order to Maximize the I_o/I_{off} ratio of a MT based on these possible molecules. Select the useful BW $< 5\text{eV}$
- (d) Identify and discuss the length L bridge derived by the optimum N rings calculated above

Question 3 - Working with the EE-BESD numerical model: details, parameters and comparisons

Here you will use EEBESD again and refer to exercise W10 for the initialization part.

EEBESD_focus1: Analysis of molecule OPE

Now analyze molecule OPE. Analyze the main features you have already analyzed for the other molecules.

EEBESD_focus1_Q1: Compare OPE to TT molecules qualitatively and quantitatively. Comment the obtained results and the difference with respect to 3TT and 4TT molecules.

EEBESD_focus2: Analysis of molecule 5TT

Change the molecule to 5TT.

EEBESD_focus2_Q2: What do you expect it will happen to the current when changing the molecule from 3TT/4TT to 5TT? Why?

EEBESD_focus2_Q3: Plot the results obtained for the 5TT molecule and compare the current trend and values to the 4TT and 3TT cases; try to associate the obtained results to the physical differences among the molecules.

EEBESD_focus2_Q4: How does the maximum number of iterations change?

EEBESD_focus2_Q5: What do you expect if we change the value of the gate voltage?

EEBESD_focus2_Q6: Try to change the gate voltage value by choosing some possible values (either using the loop or just running the script a few times). Use values that are meaningful and could change the molecule toward a HOMO type or a LUMO type.

Warning: concerning the transmission spectrum plot, carefully read the MATLAB code to understand what EE-BESD plots and eventually modify the code to analyze the gate voltage effects correctly.

EEBESD_focus2_Q7: Evaluate the best I_{on}/I_{off} ratio you can get with this molecule.

Remark: the I_{off} current is defined as the current flowing from the drain to source when the gate voltage is zero. Ideally, this value should be 0, but due to several parasitic effects (e.g. quantum tunneling between gate and channel in standard FET), it is not. The I_{on} current is defined as the current flowing from drain to source when gate and drain are connected to the supply voltage

(saturation current) and the source to the ground potential. The ratio between I_{on}/I_{off} is called *Applicability*, and it is very interesting from the electronic point of view.

Another interesting aspect of the molecular transistor is related to the actual evolution of molecule peaks when changing the drain-source voltage. In the folder 5TT, a file named “TS_5tt.au.txt” is provided. It contains the TS for several values of V_{ds} . The TS are shown in figure 3.

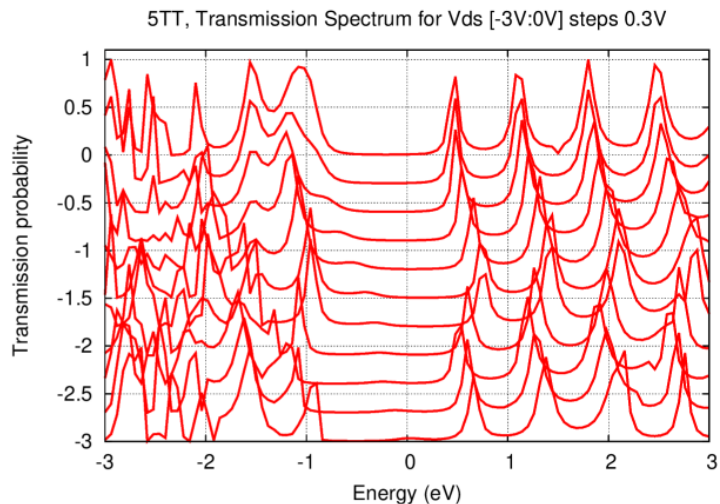


Figure 3: TS of 3-rings thiophene molecule for V_{ds} changing from 0 (top graph) to -3V (bottom graph); variations are 0.3V from one graph to the next.

EEBESD_focus2_Q8: A shift tendency in the peak associated to the LUMO can be observed. How do you explain it?

EEBESD_focus3: Analysis of the OPV molecule

Now analyze the OPV molecule. Analyze the main features you have already analyzed for the other molecules. Change the parameters and observe the possibilities for this molecule.

EEBESD_focus3_Q9: Compare and comment on the differences among OPV to OPE molecules, qualitatively and quantitatively.

EEBESD_focus3_Q10: Try to model the presence of a Back-gate in the system and test a few cases. Study the relation between the gate and the back-gate.

EEBESD_focus3_Q11: Which is the best molecule to be used as a transistor for digital purposes?

EEBESD_focus3_Q12: Which is the best molecule to be used as a transistor for analog purposes? (look at the G calculated after the current, derive and plot the I_{DS} vs V_{GS} curve)

Warning: the plot of the current might be slightly noisy when varying the V_{GS} , making difficult the evaluation of the current derivative. This effect is caused by low numerical precision and it can be understood by carefully analyzing the EE-BESD code. To reduce this effect, increase the algorithm precision, enabling evaluating the current on a denser number of energy points (see the energy vector in “*EeBesdStandard.m*”).

EEBESD_focus4: OPTIONAL: Analysis of molecule 3TT

In this exercise, you are required to go deeper into the EE-BESD code, modifying it to obtain some additional information.

EEBESD_focus4_Q13: OPTIONAL: Consider two different values of V_{ds} : a small one, e.g. $V_{ds,A} = 0.1$ V, and a larger one, e.g. $V_{ds,B} = 2.5$ V. Execute the algorithm separately using these two values of V_{ds} . In each case, save in an array the progressive values of N (or N-N0) (N0=N_electrons) and of E1 (or Uscf) and plot them. Did you expect the obtained trend with $V_{ds,A}$ and $V_{ds,B}$?