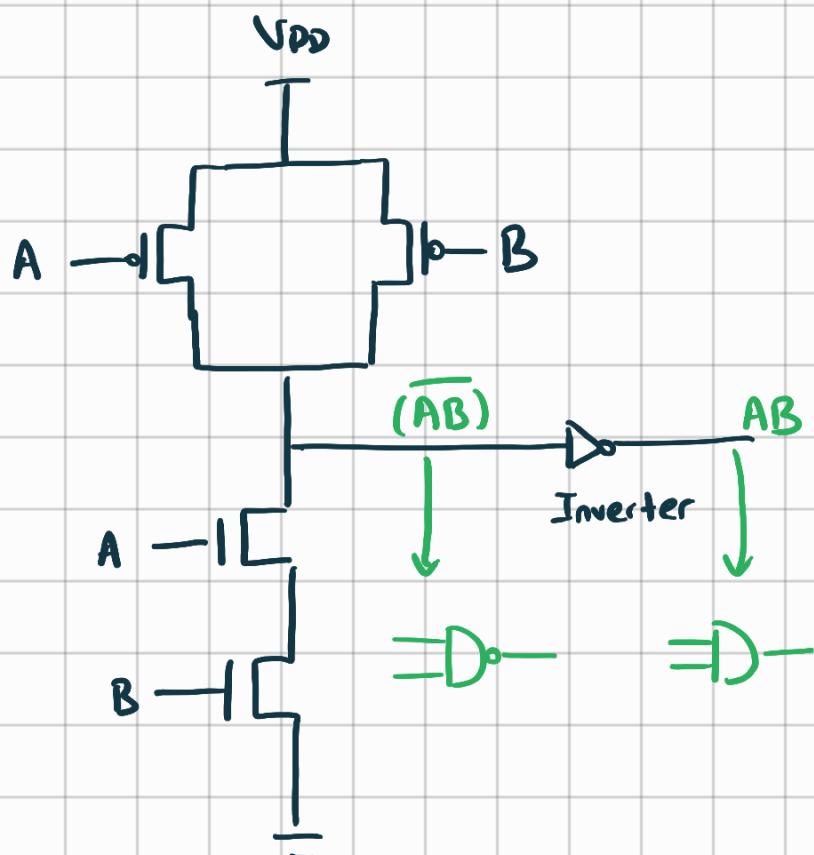
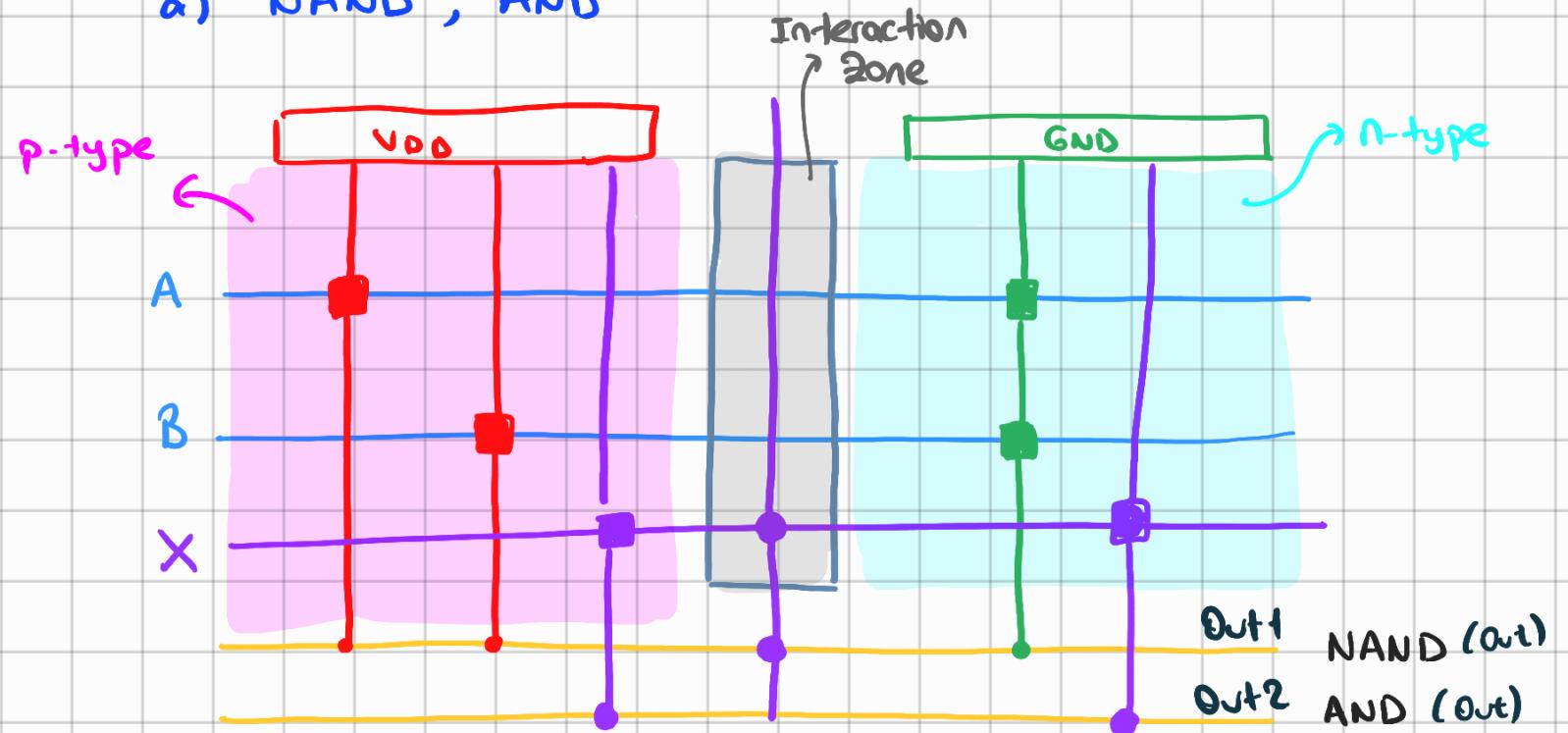


Question 1 Array Circuits with Molecular Transistors

a) NAND, AND



- Explain current flow depending on input conditions

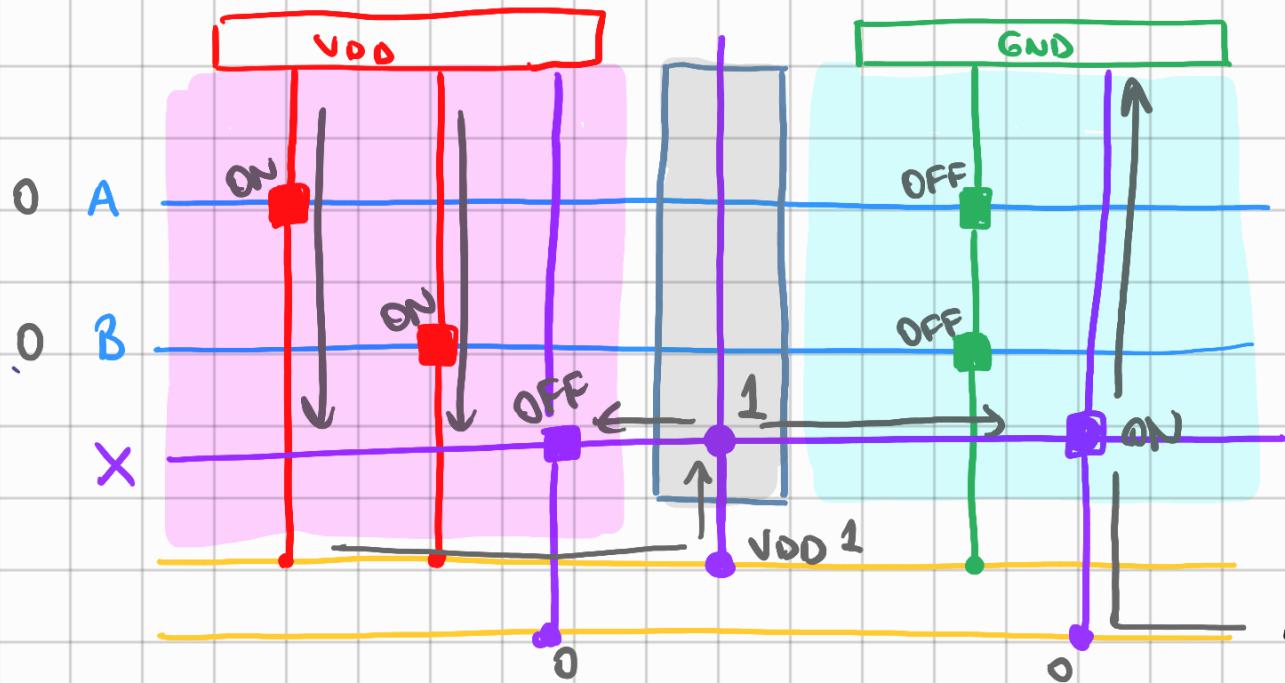
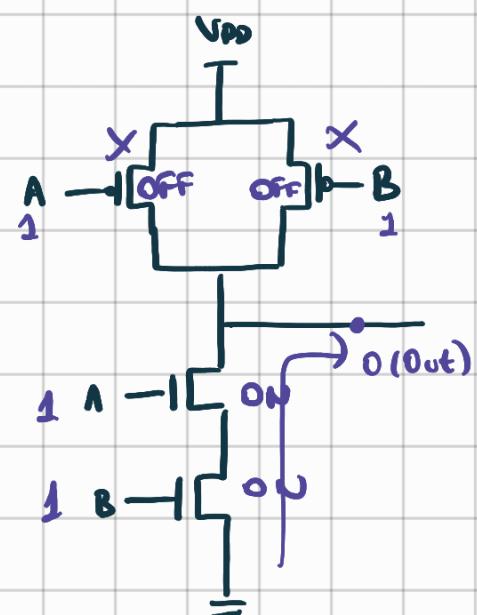
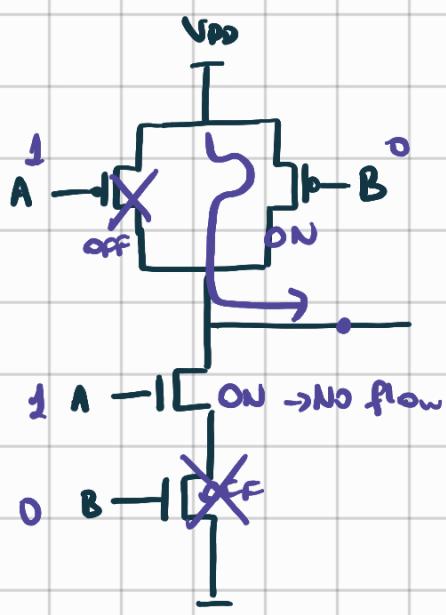
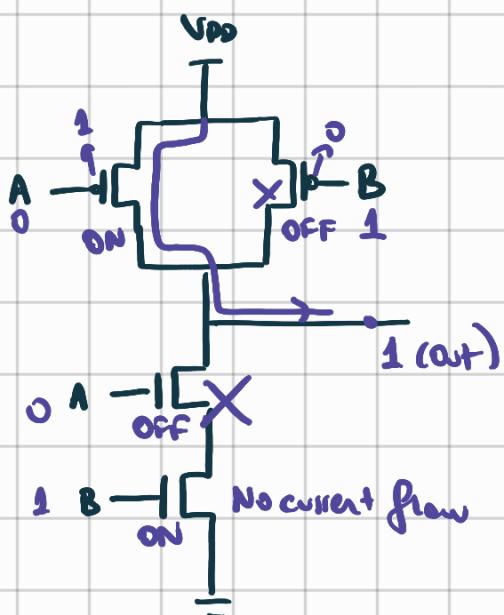
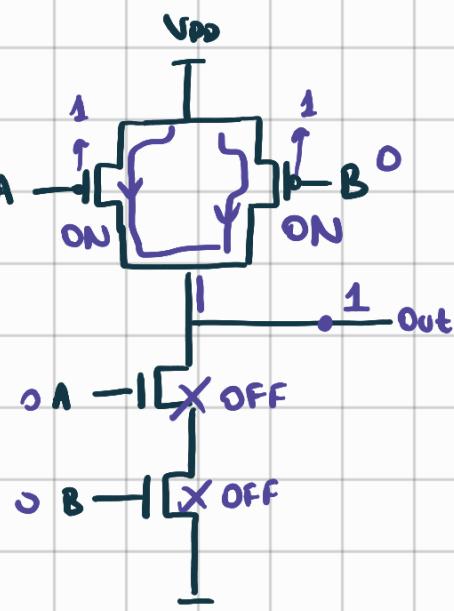
- Verify the truth table.

- Discuss where problems could arise

Truth Table NAND & AND

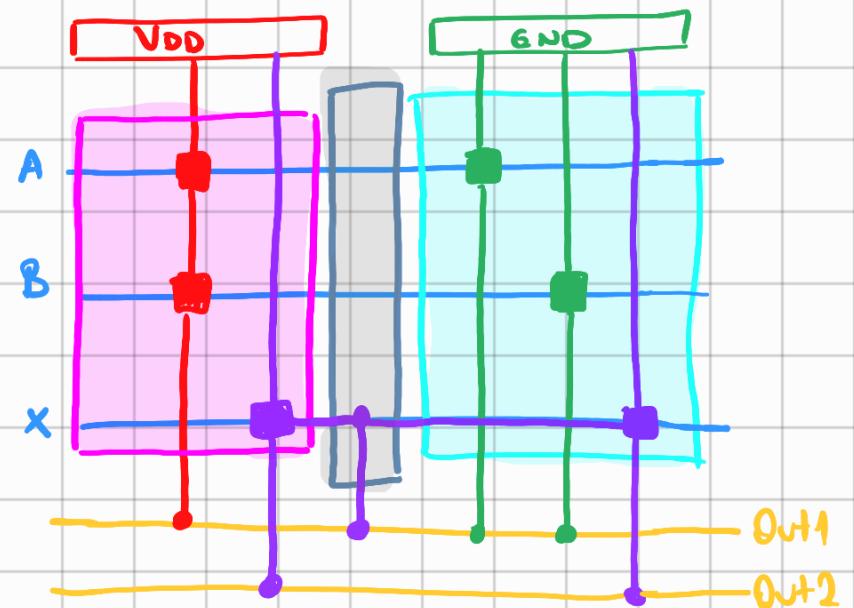
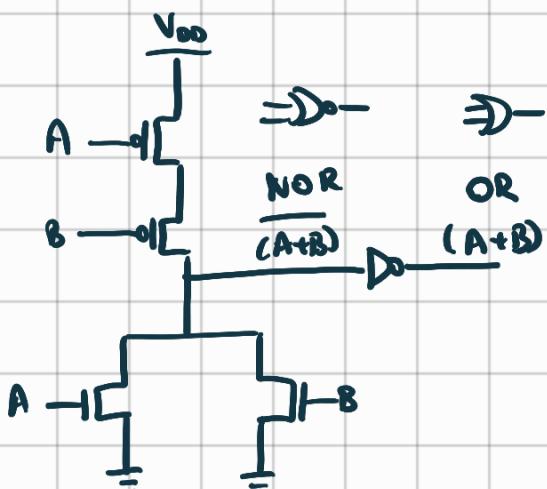
		(Out1)	(Out2)
		Out1	Out2
A	B		
0	0	1	0
0	1	1	0
1	0	1	0
1	1	0	1

Invert



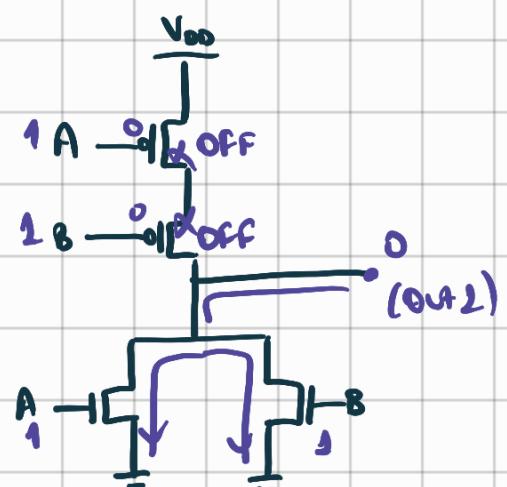
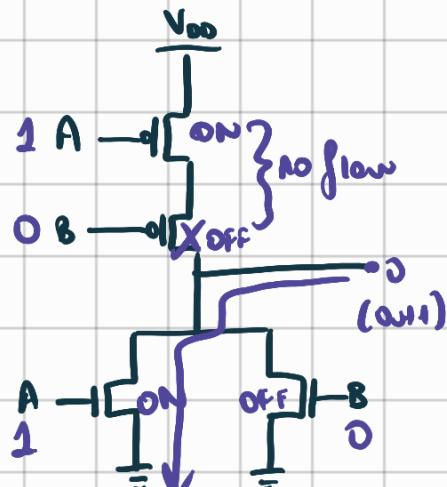
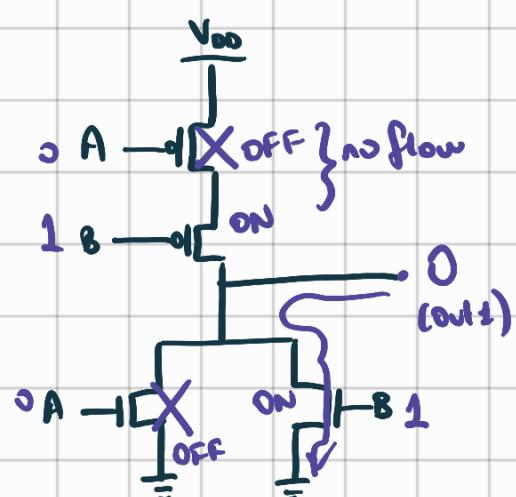
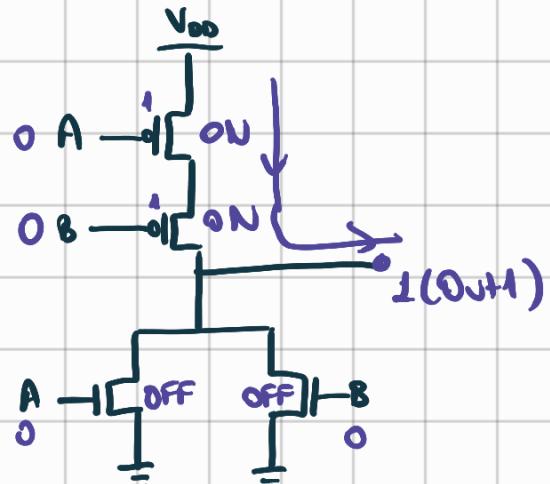
(1)
NAND (Out)
AND (Out)
(0)

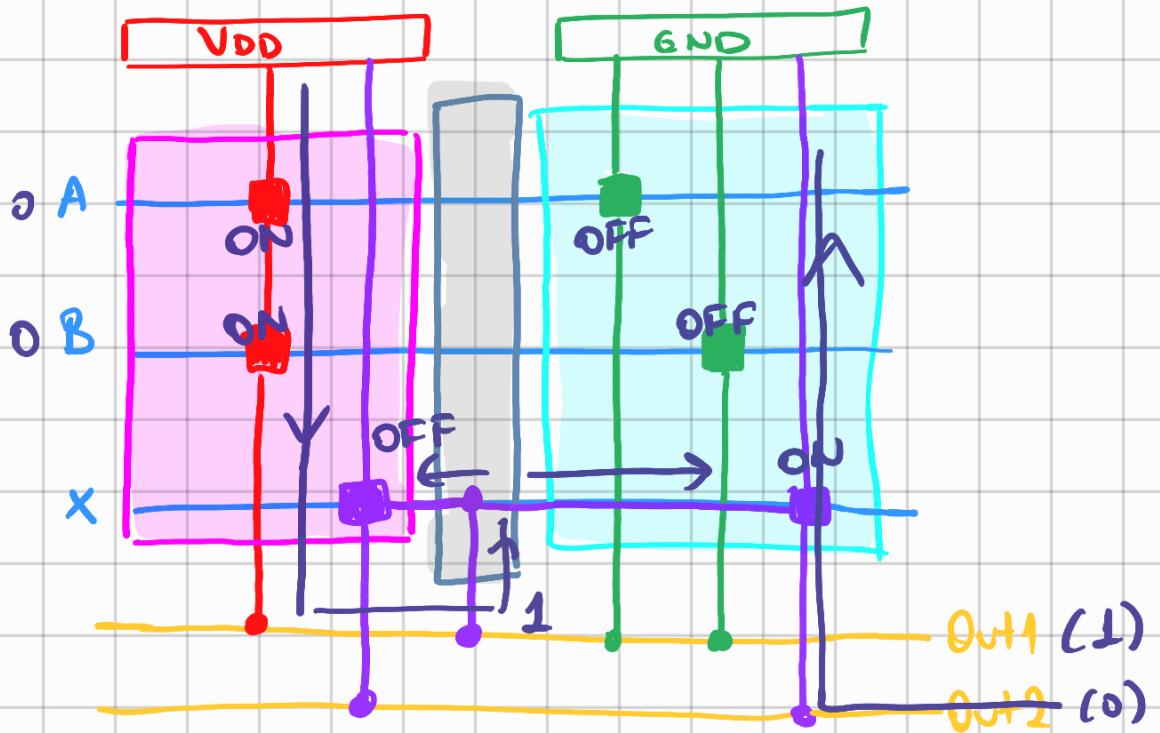
b) NOR, OR



Truth Table for NOR & OR

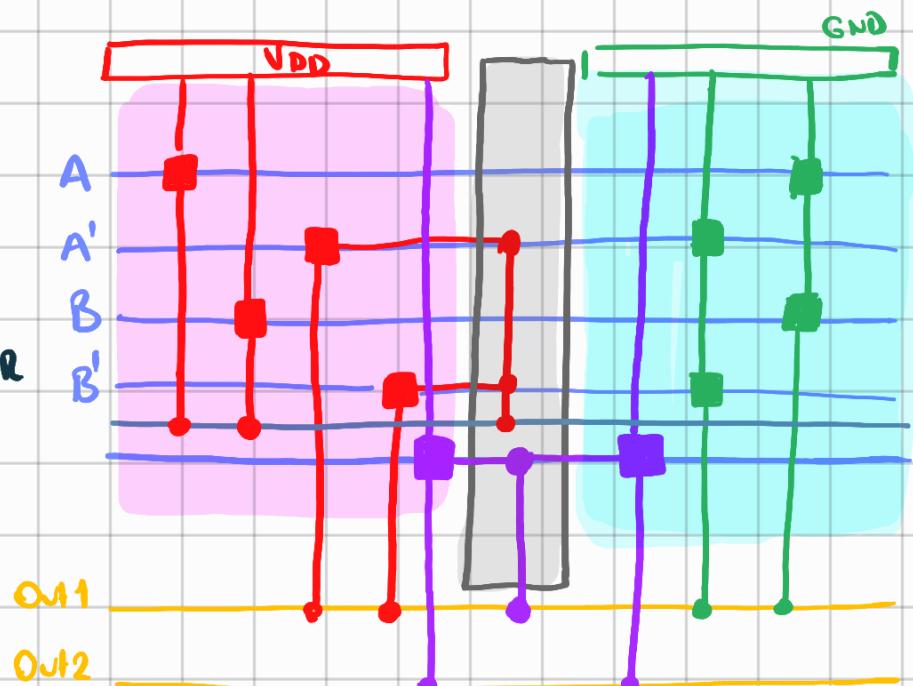
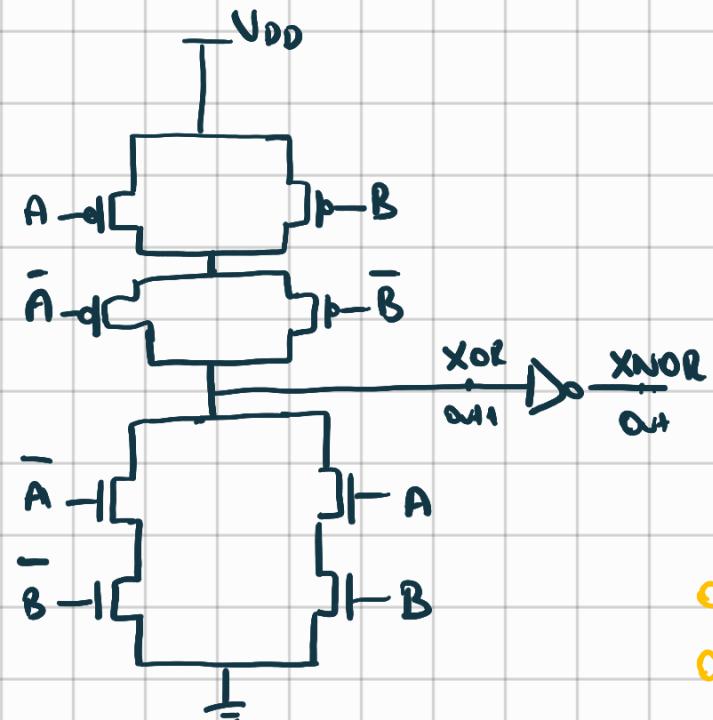
A	B	(NOR)		(OR)	
		Out1	Out2	Out1	Out2
0	0	1	0	0	1
0	1	0	1	1	1
1	0	0	1	1	0
1	1	0	1	1	0





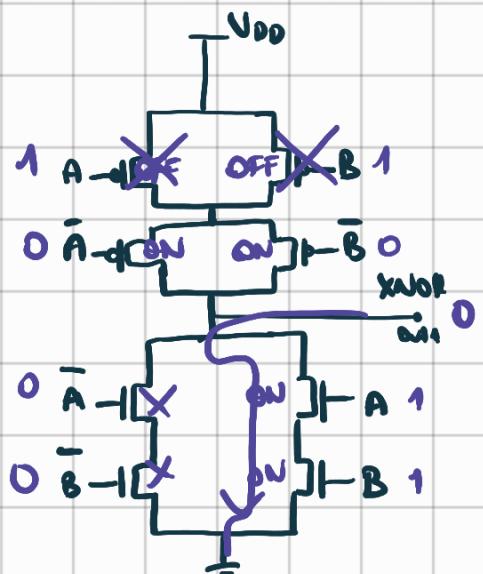
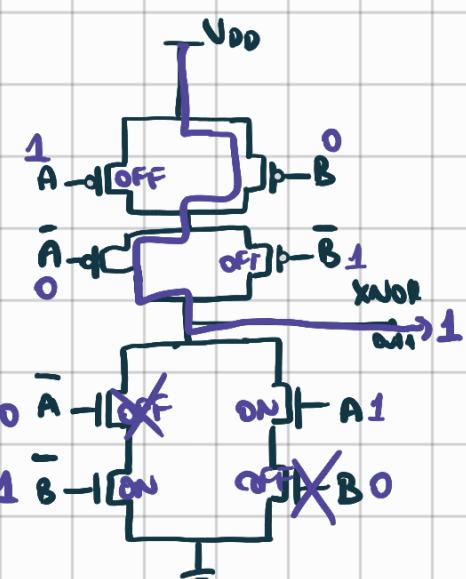
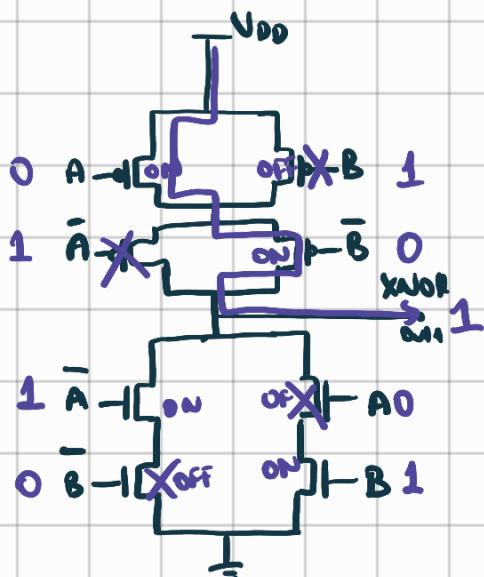
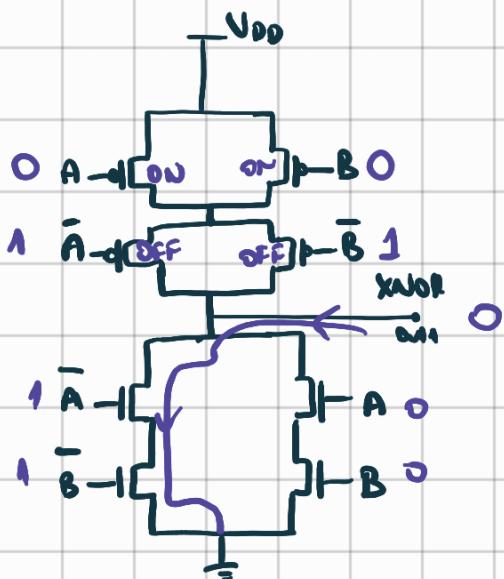
c) XOR, XNOR

$$\text{XOR} = A\bar{B} + \bar{A}B, \text{XNOR} = \bar{A}\bar{B} + A\bar{B}$$



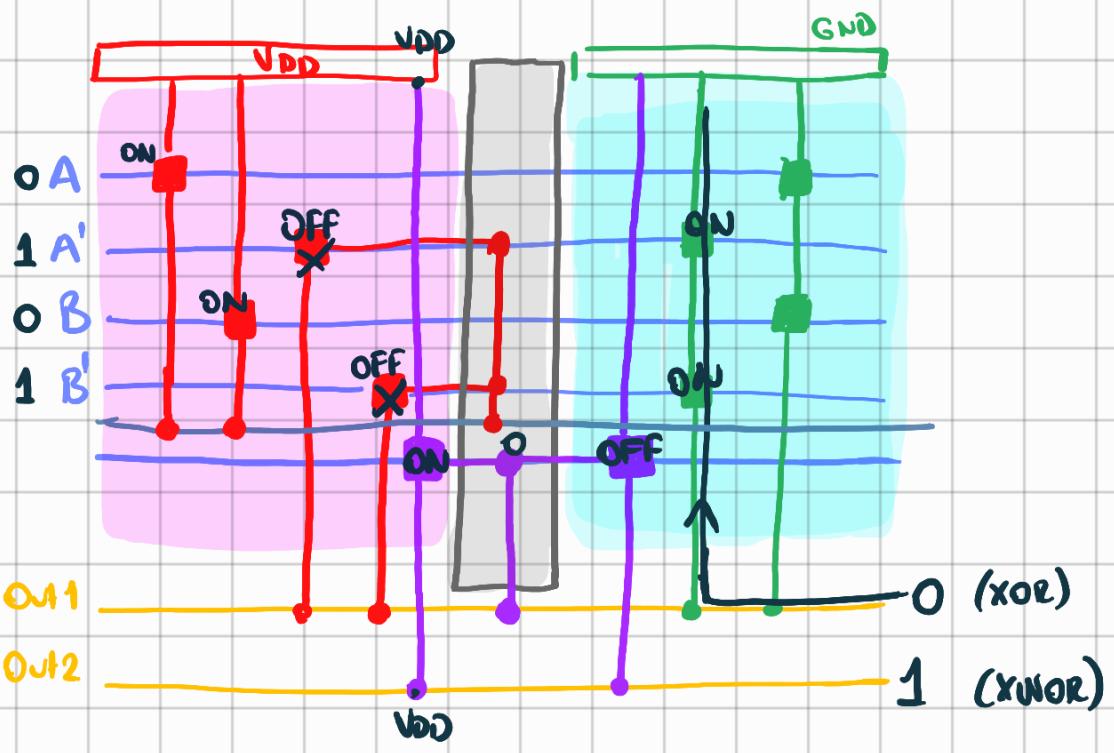
Truth Table for XOR XNOR

A	B	XOR	XNOR
		Out1	Out2
0	0	0	1
0	1	1	0
1	0	1	0
1	1	0	1



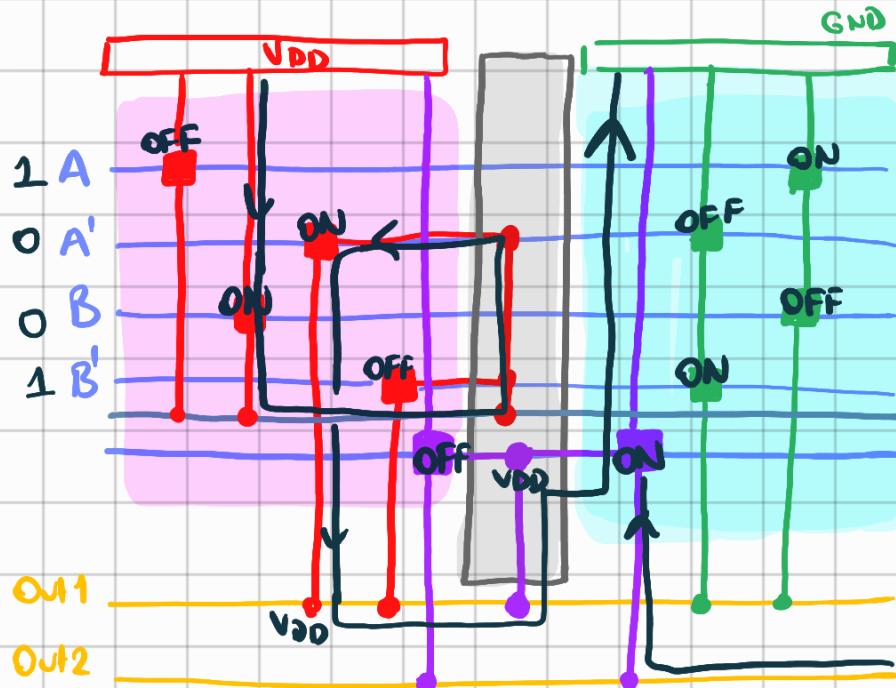
Case 1

$$A=B=0$$

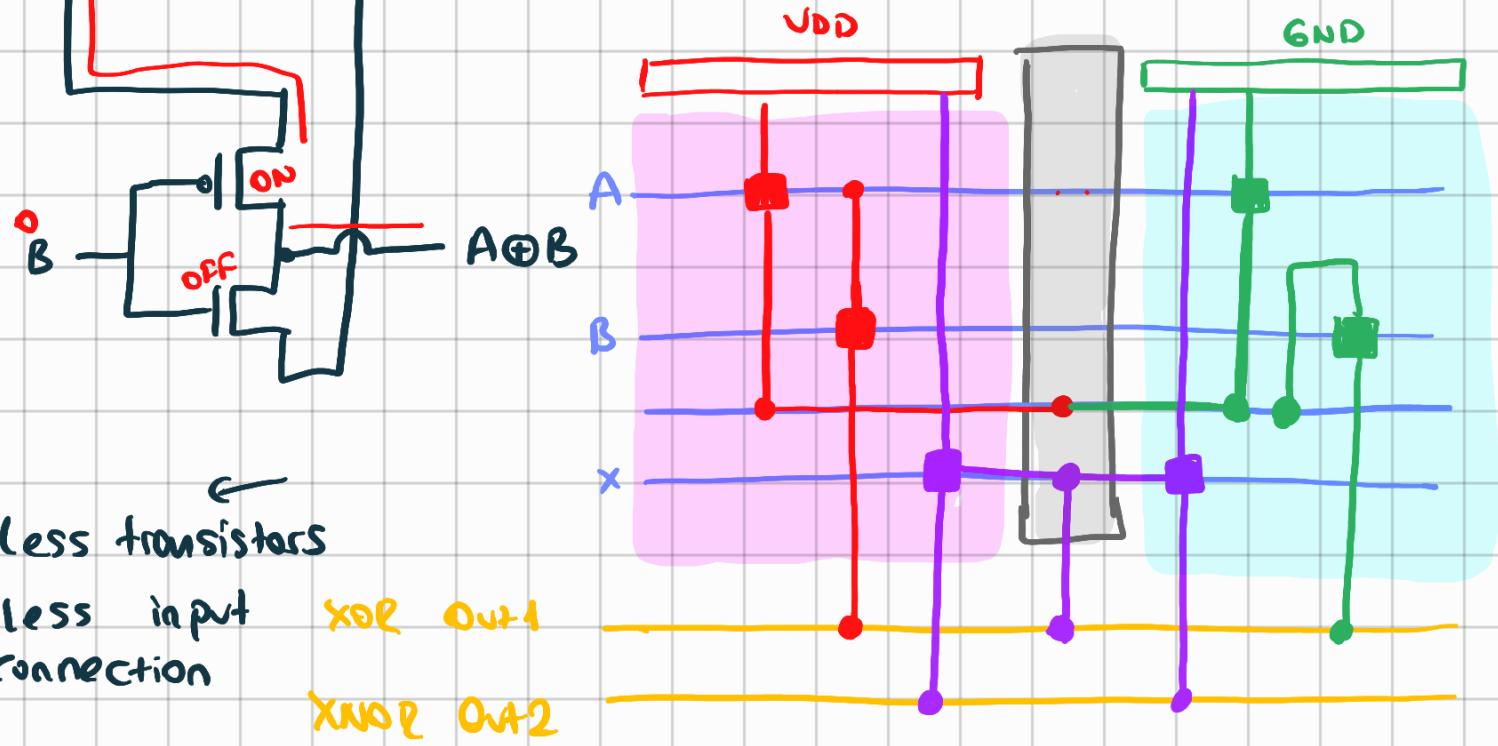
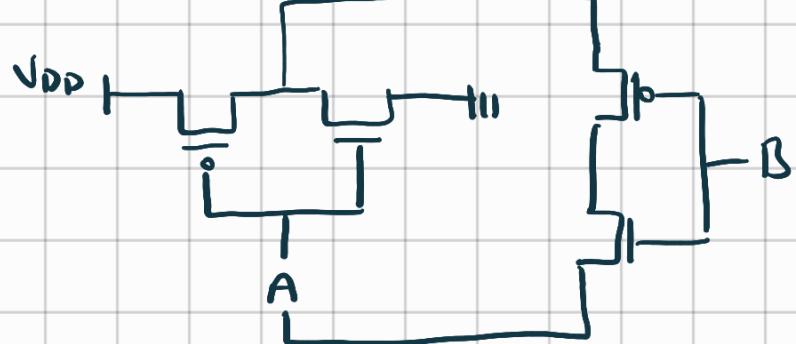
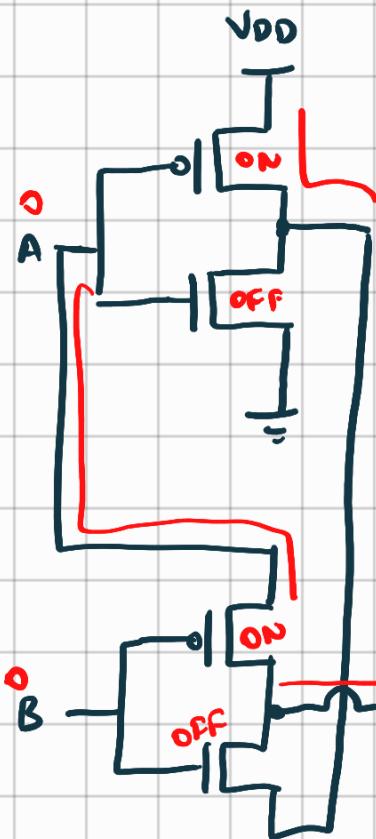


case 2

$$\begin{aligned} A &= 1 \\ B &= 0 \end{aligned}$$



More Basic Design

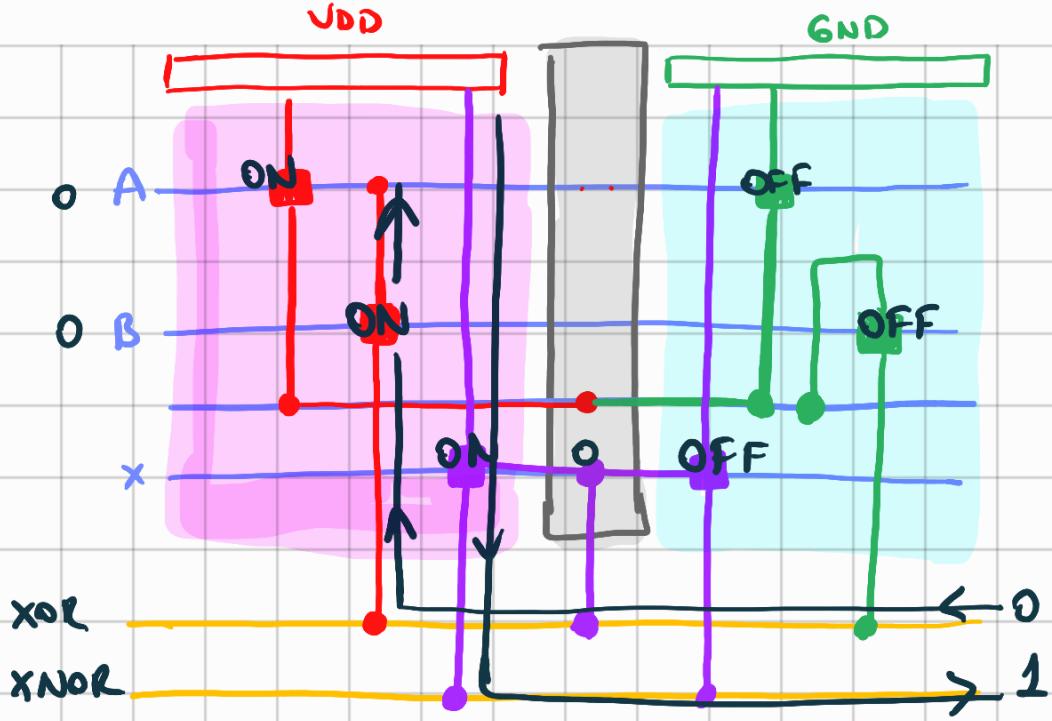


↳ less transistors

* less input connection
XOR OUT1
XNOR OUT2

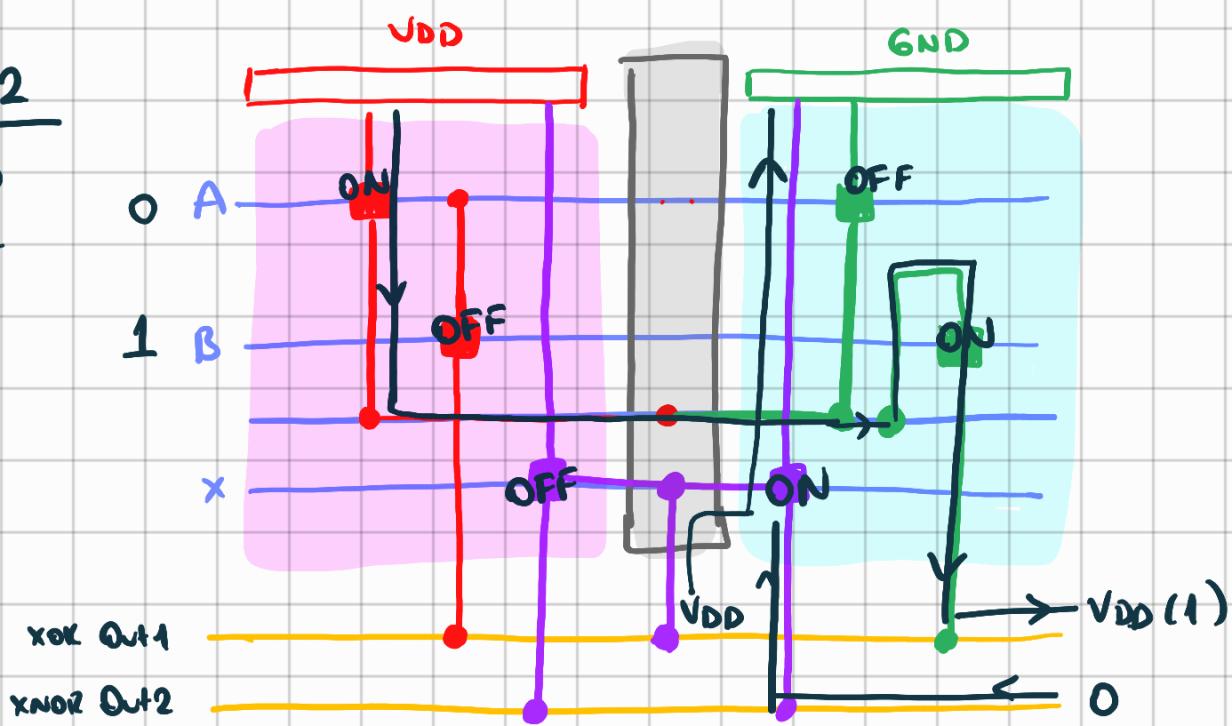
Case 1

$A=0$
 $B=0$

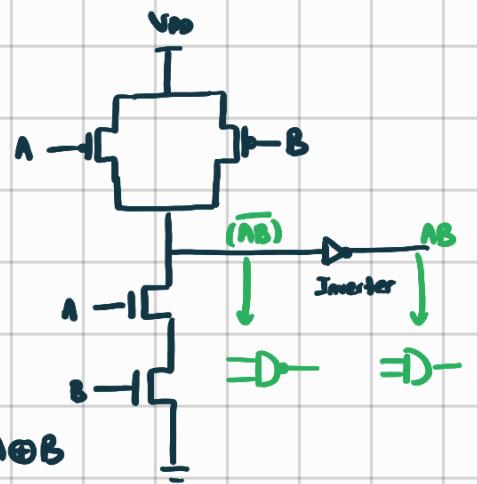
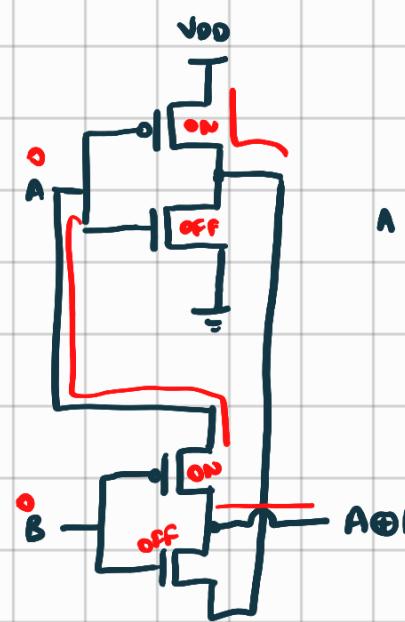
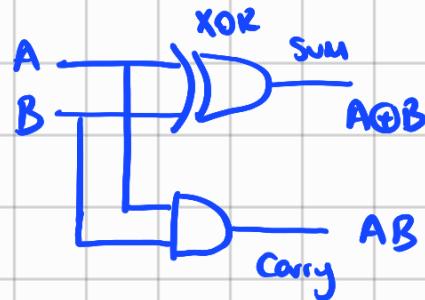


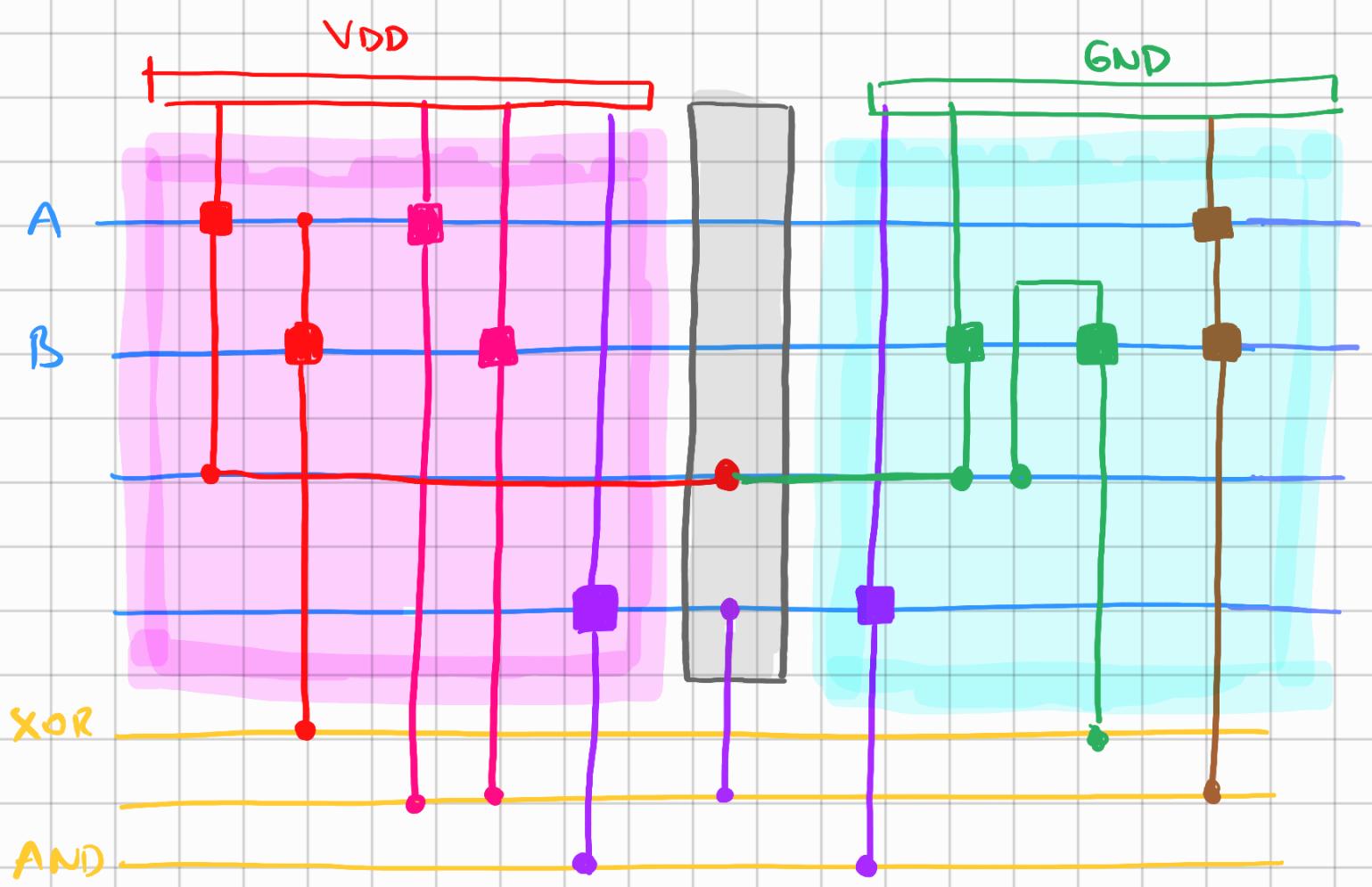
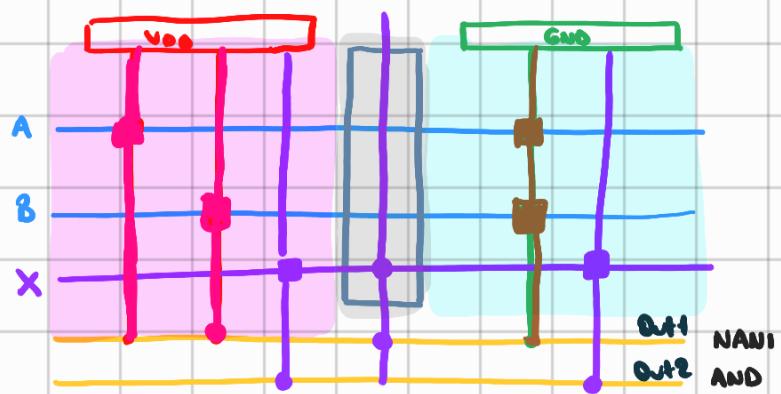
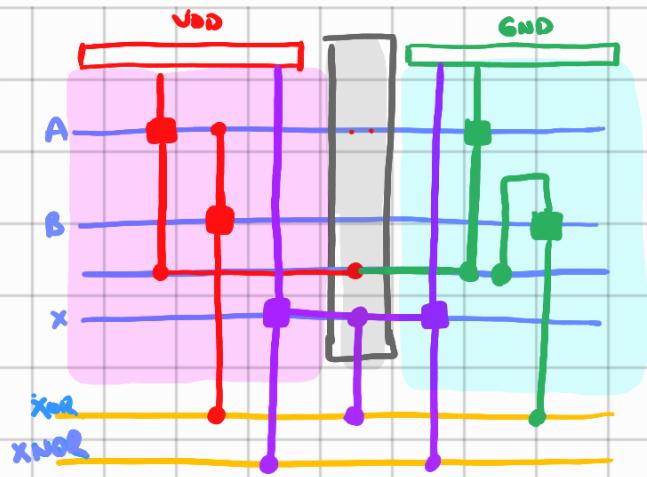
Case 2

$A=0$
 $B=1$



d) Half adder

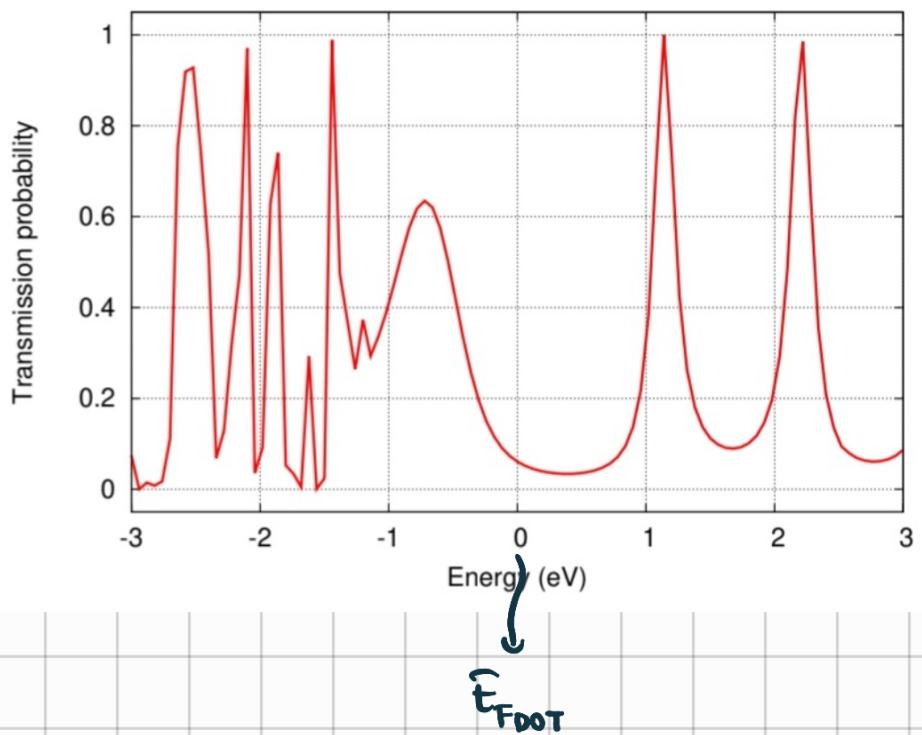




Question 3 → focus 1

An initial analysis of 3TT Molecule

3TT, Transmission Spectrum @Equilibrium



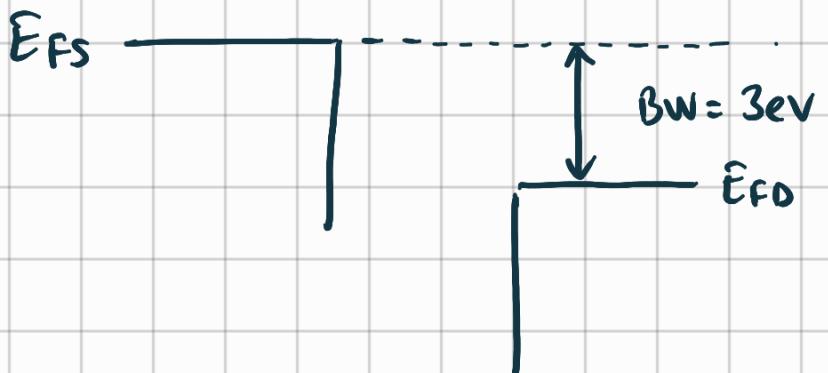
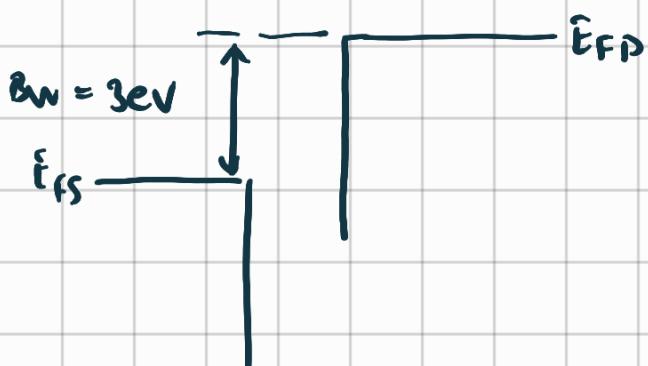
Focus 1. Q1)

$$BW = E_{FS} - E_{FD} = qV_{DS}$$

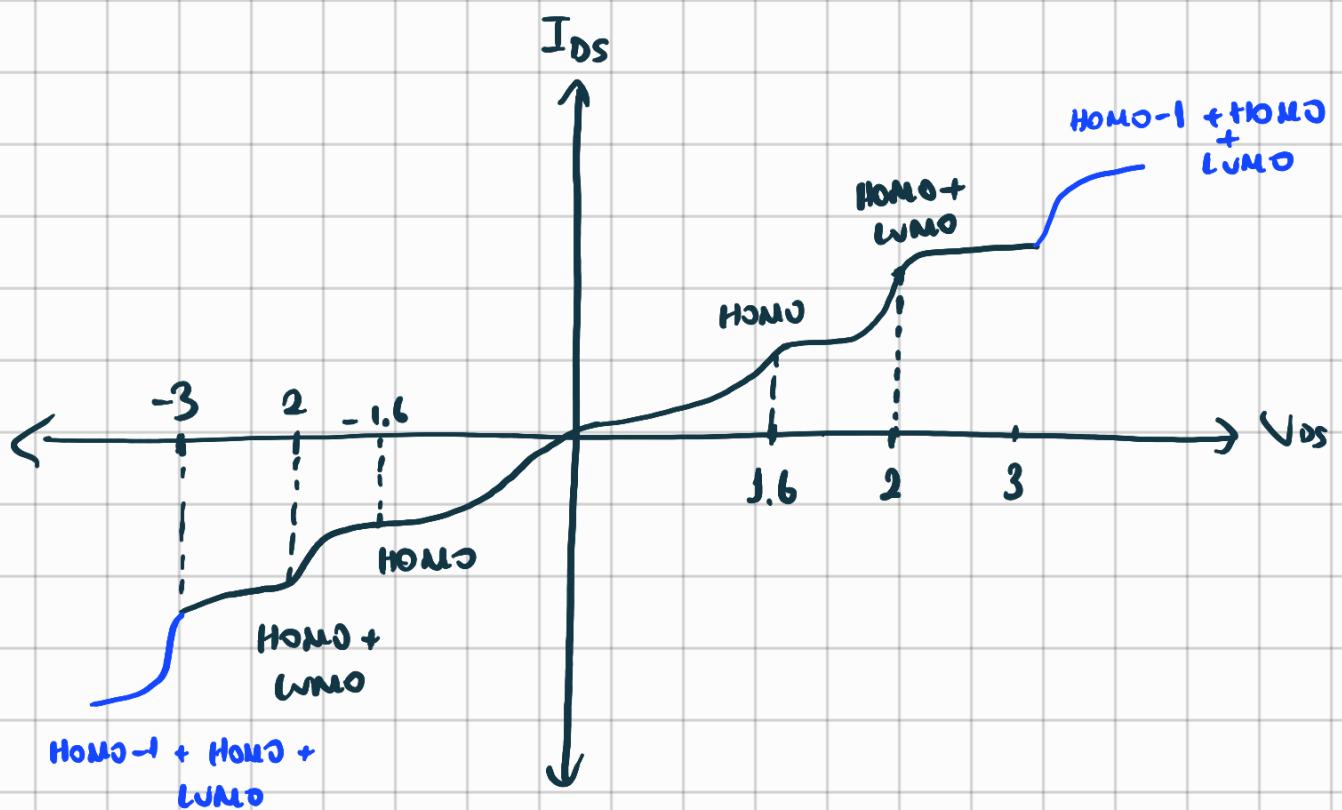
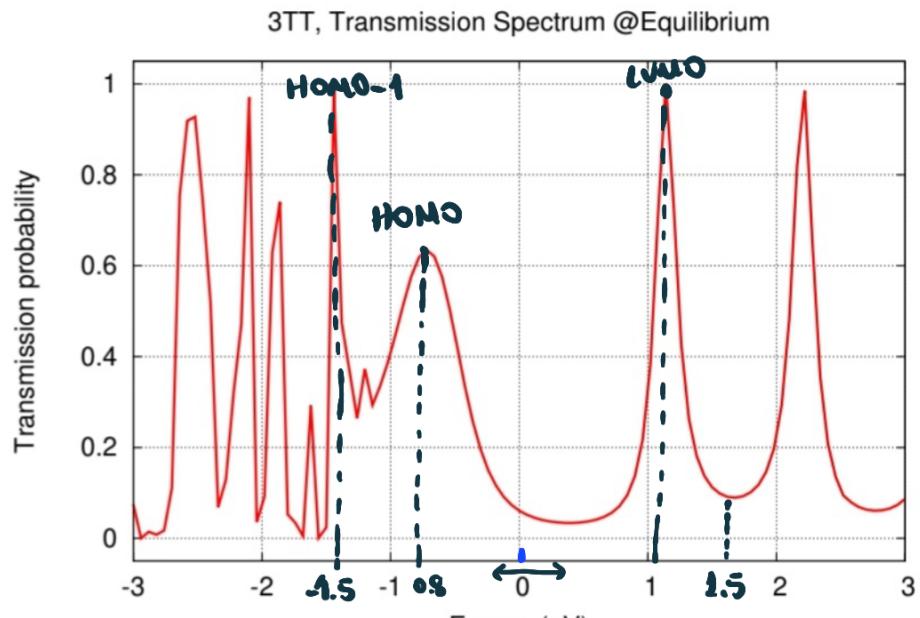
for $V_{DS} = [-3V, +3V]$



the maximum width of
 $BW = 3\text{eV}$ when $V_{DS} = +3V$
 or $V_{DS} = -3V$.

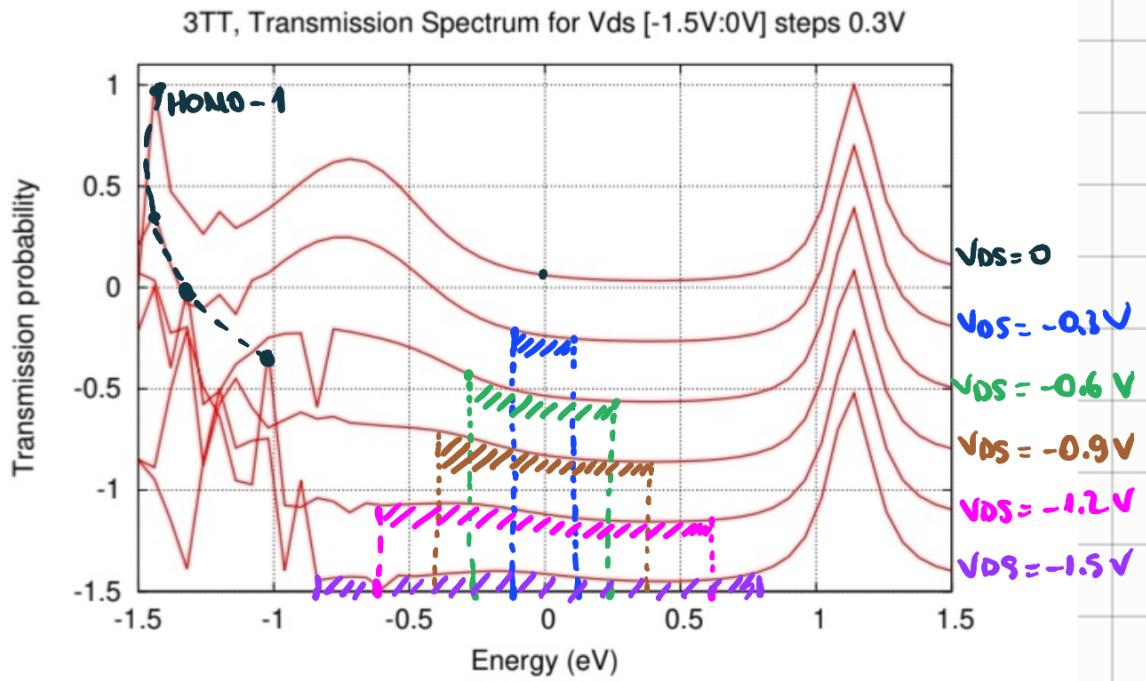


Focus1 Q2



Here we assumed, TS (transmission spectrum is fixed)

Focus 1 Q3

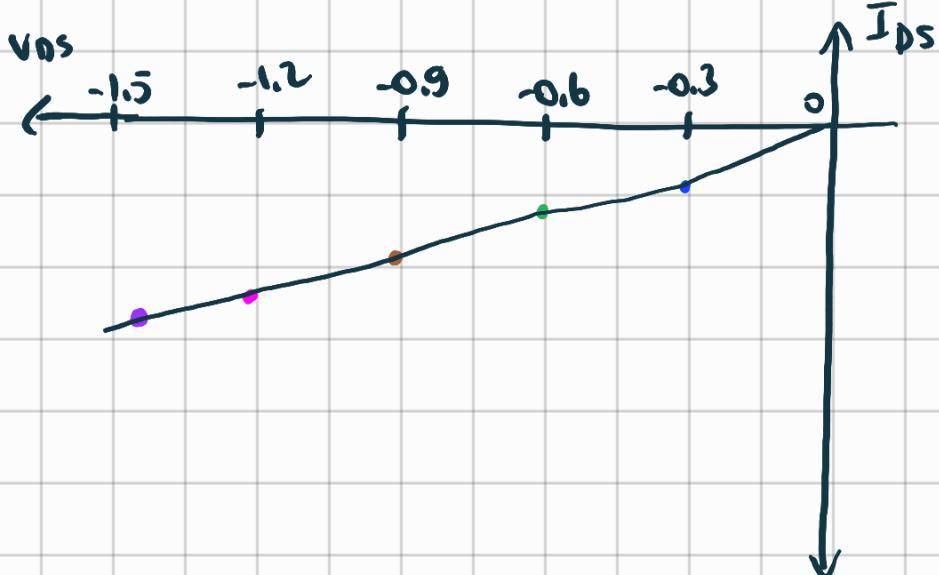


$$V_{DS} = -q \frac{C_D}{C_S} V_{DS}$$

$V_{DS} < 0$ $V_{DS} > 0$ shifts higher energies

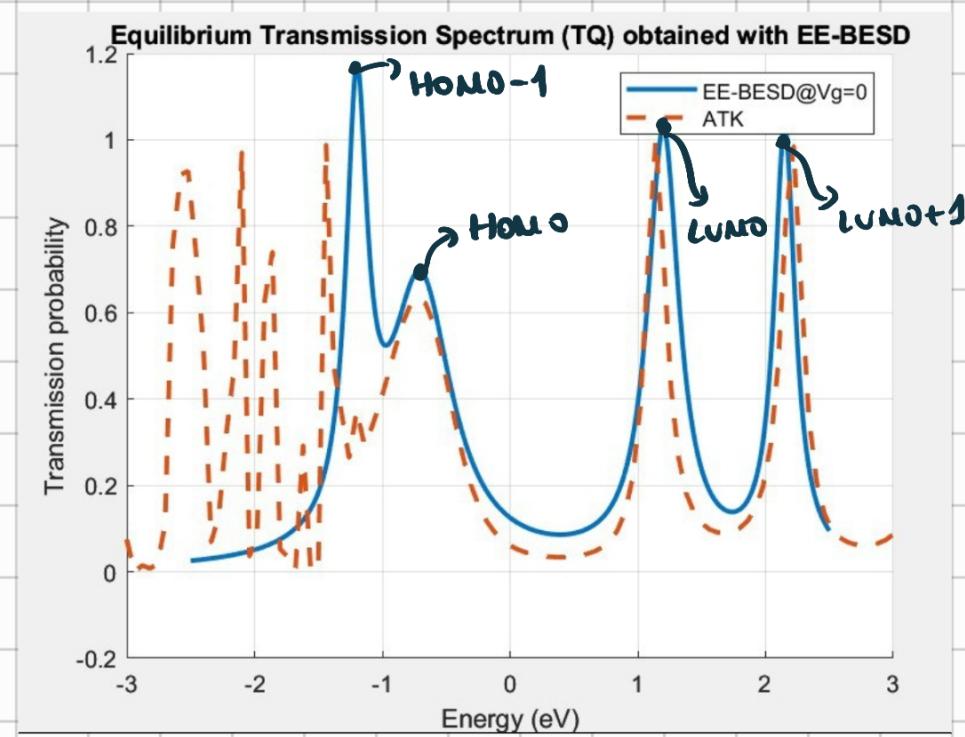
Spectra shifted towards higher energies. And HOMO-1 also participates to conduction.

Focus 1 Q4



Focus 1 Q5

$$E_0 = [-0.7 \quad -1.2 \quad 1.2 \quad 2.15] \rightarrow \text{energy levels}$$



Focus 1 Q6

Parameters :

$q = 1\text{e}^-$ charge (Coulombs)	$G_0 = \text{conductance } (?)$
$h = \text{Planck constant } (\text{Js})$	$k = \text{Boltzmann constant}$
$\hbar = \text{Reduced planck constant } (\text{Js})$	$T = \text{temperature } (\text{°C})$
$m = e^- \text{ mass } (\text{kg})$	$kT = k(T + 273)/q \text{ eV}$
$\epsilon_0 = \text{Vacuum permittivity } (\text{F/m})$	

$U_F = 0$ Fermi energy level of DOT

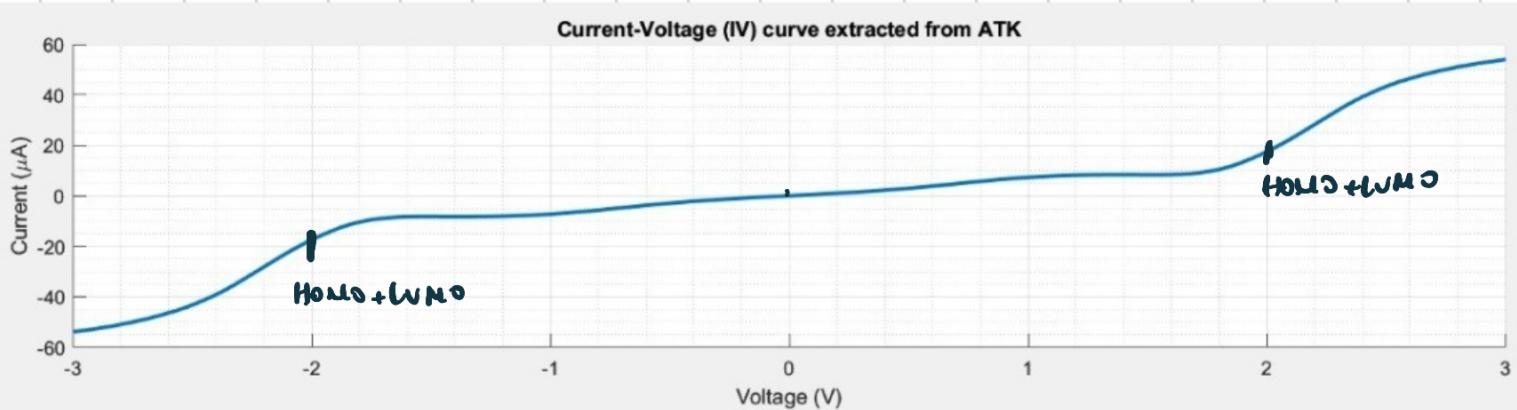
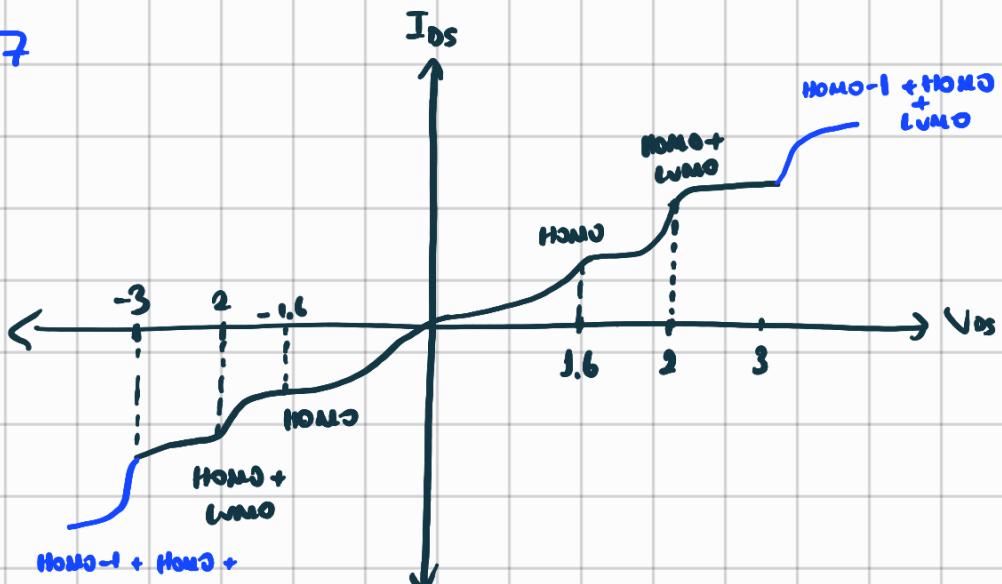
\tilde{E}_0 = energy levels [HOMO-1, HOMO, LUMO, LUMO + 1]

γ_1 = coupling factor between electrode and molecule ^{source}

γ_2 = coupling factor between drain and molecule

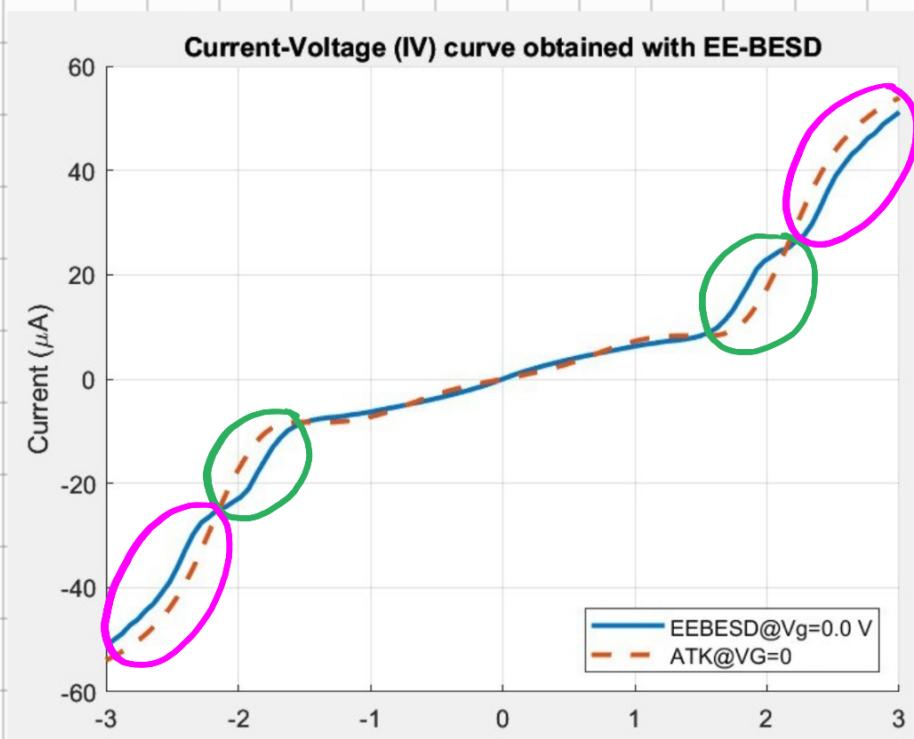
$\gamma = \gamma_1 + \gamma_2$ = total coupling factor ?

Focus 1 Q7

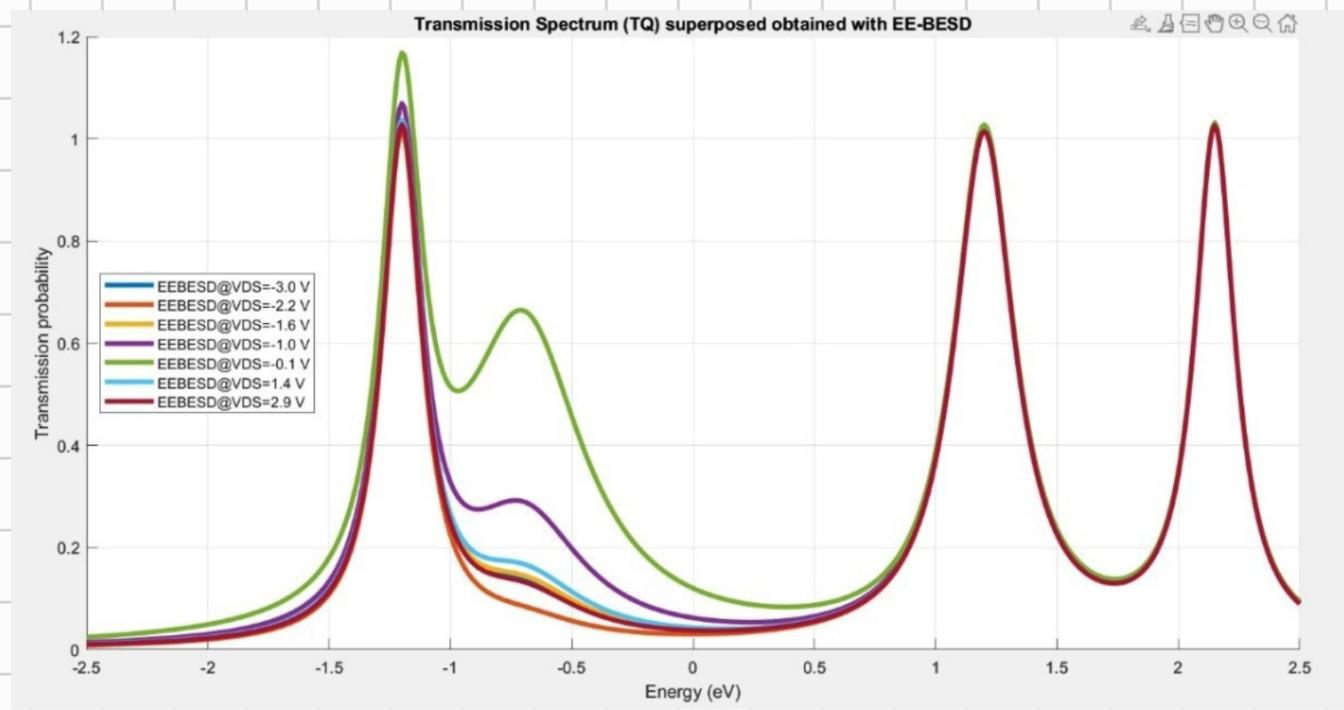


They look similar.

Focus 1 Q8



Focus 1 Q9

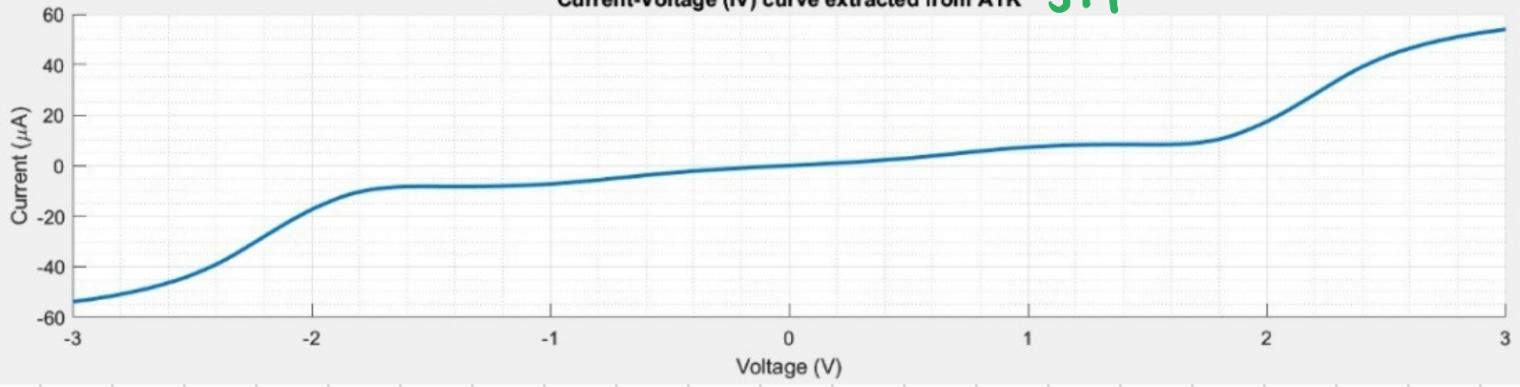


There's a considerable difference between EEBESD & ATK in peak variations. For EEBESD, lower energy levels than HOMO-1 are not present.

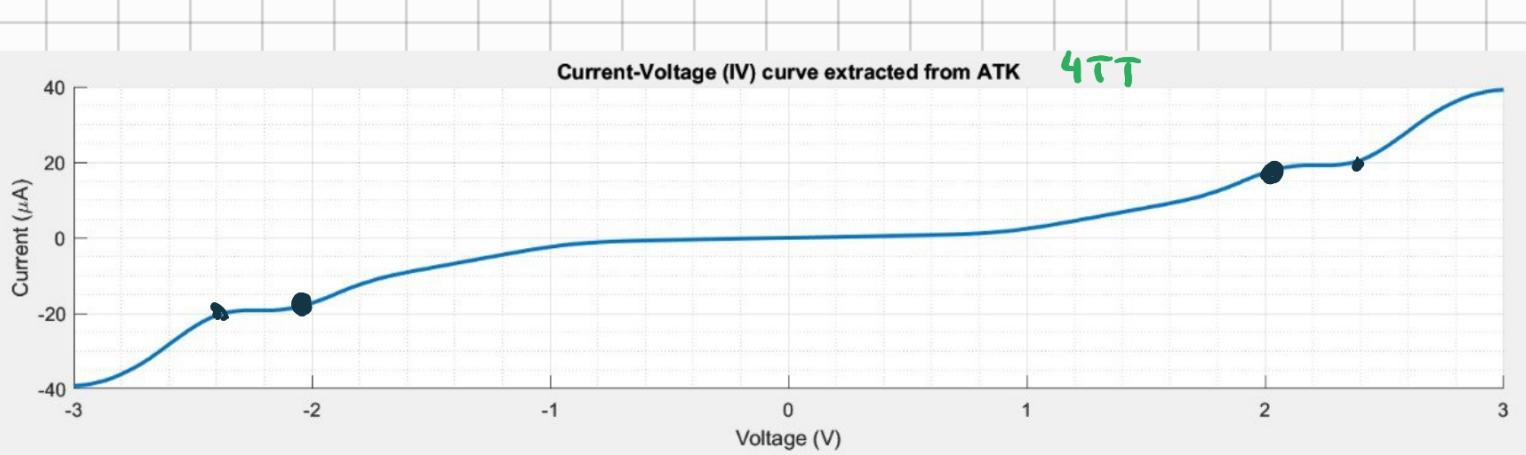
Focus 2

Q10

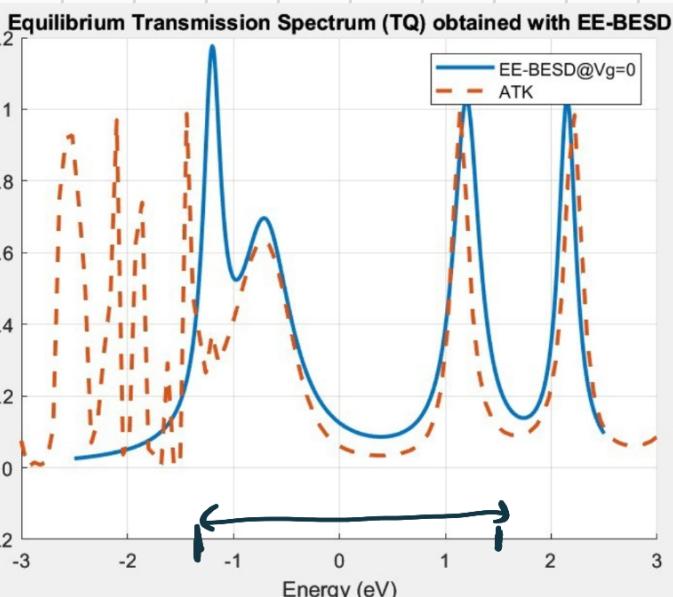
Current-Voltage (IV) curve extracted from ATK 3TT



Current-Voltage (IV) curve extracted from ATK 4TT

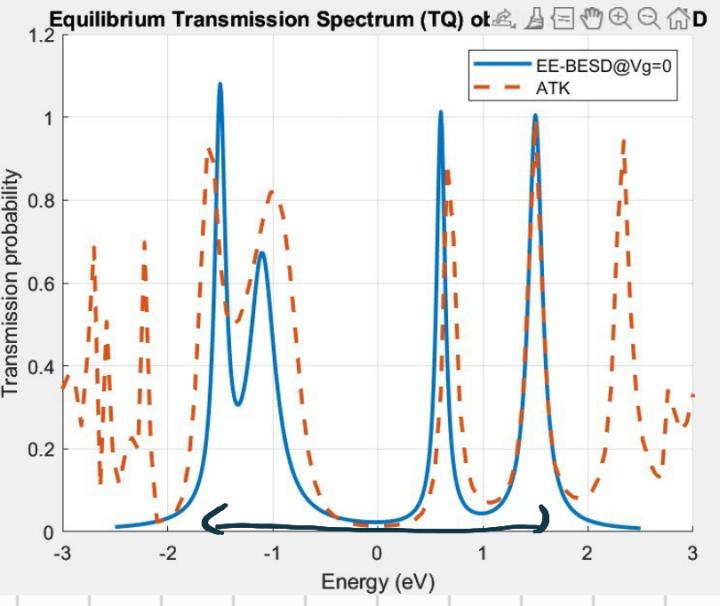


For 3TT case, current is larger than 4TT.



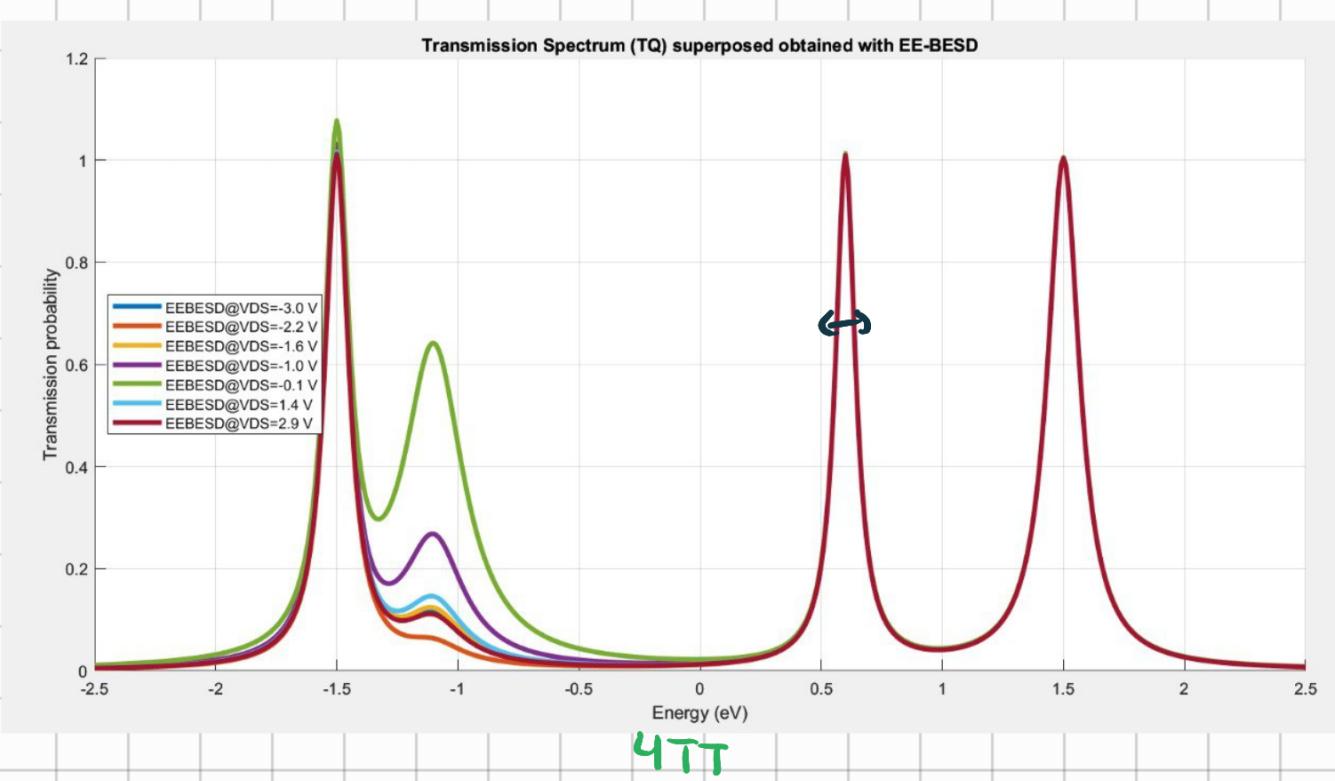
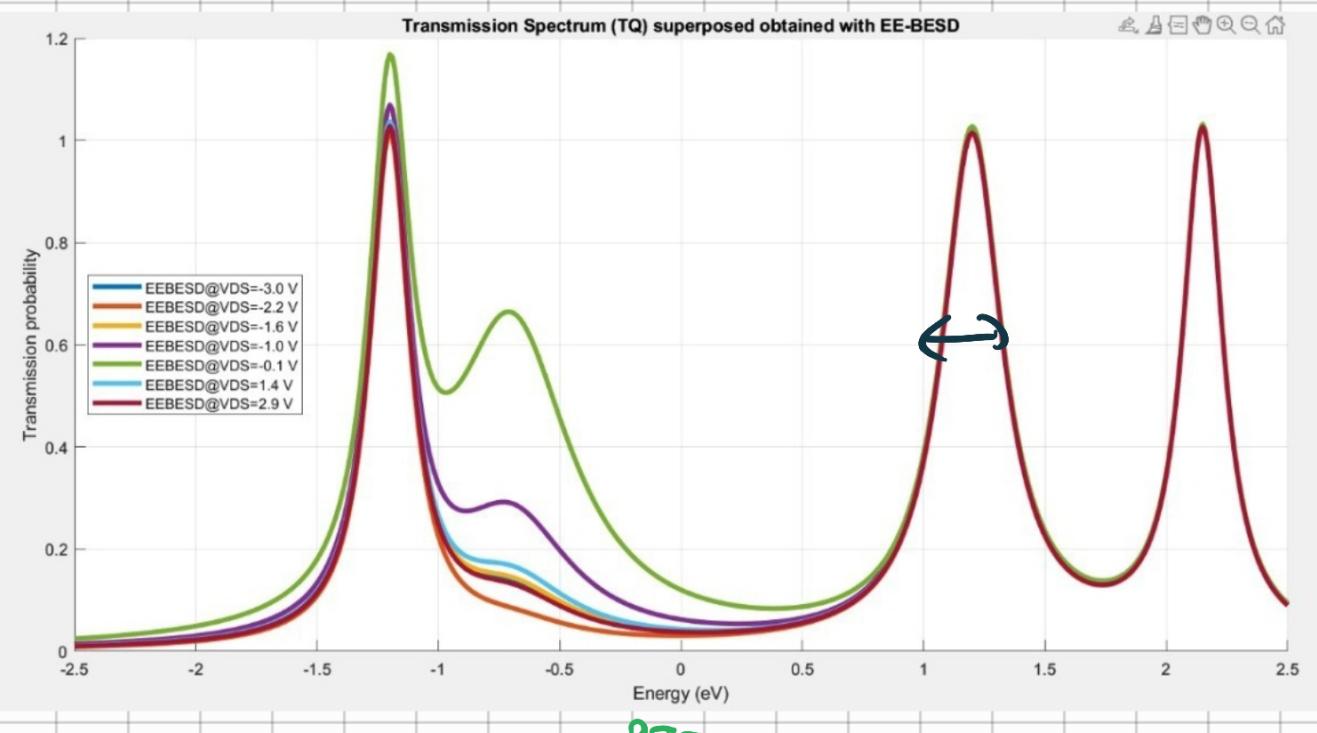
3TT

3 peaks



4TT

4 peaks



For 4TT, broadening is reduced; thus, narrow peaks occur and these factor decreases I_{DS} . Even though more peaks and reduction in HLG occur.

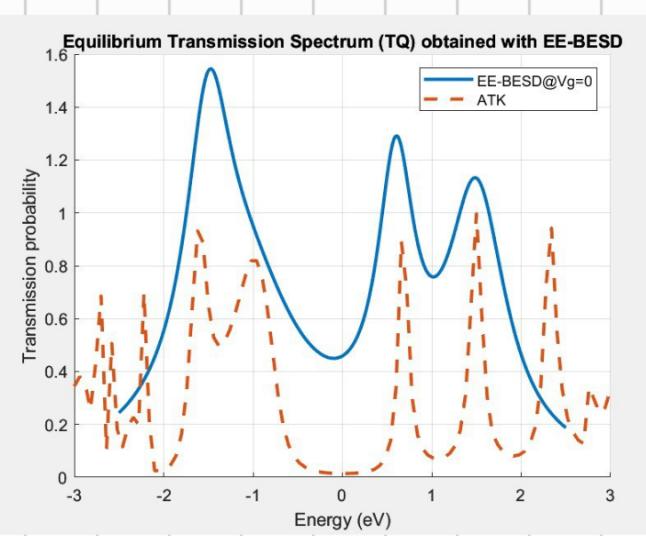
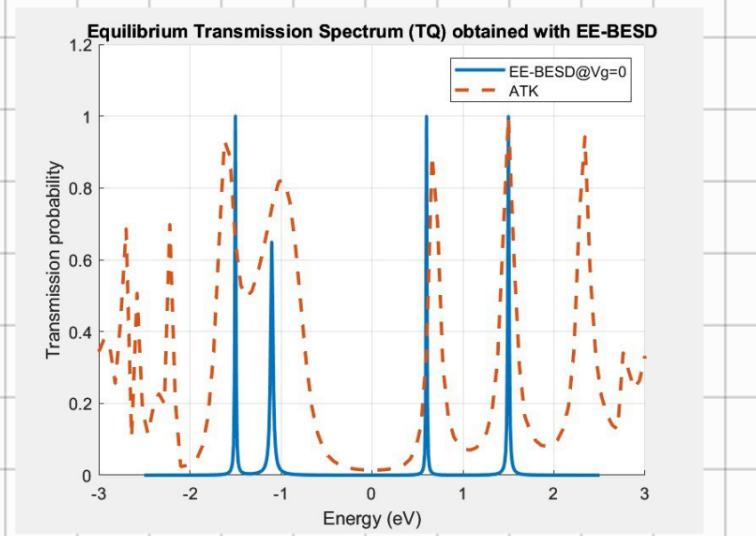
Focus 2 Q11

Expectations:

Decreasing coupling factor yields weaker bonding; therefore, narrow peaks are expected. (broadening decreases). Thus, smaller current values are expected.

Increasing coupling factor yields stronger bonding \Rightarrow

Increased broadening \rightarrow wider peaks \rightarrow Increase in current



$$\gamma = 0.01$$

$$\gamma = 0.5$$

