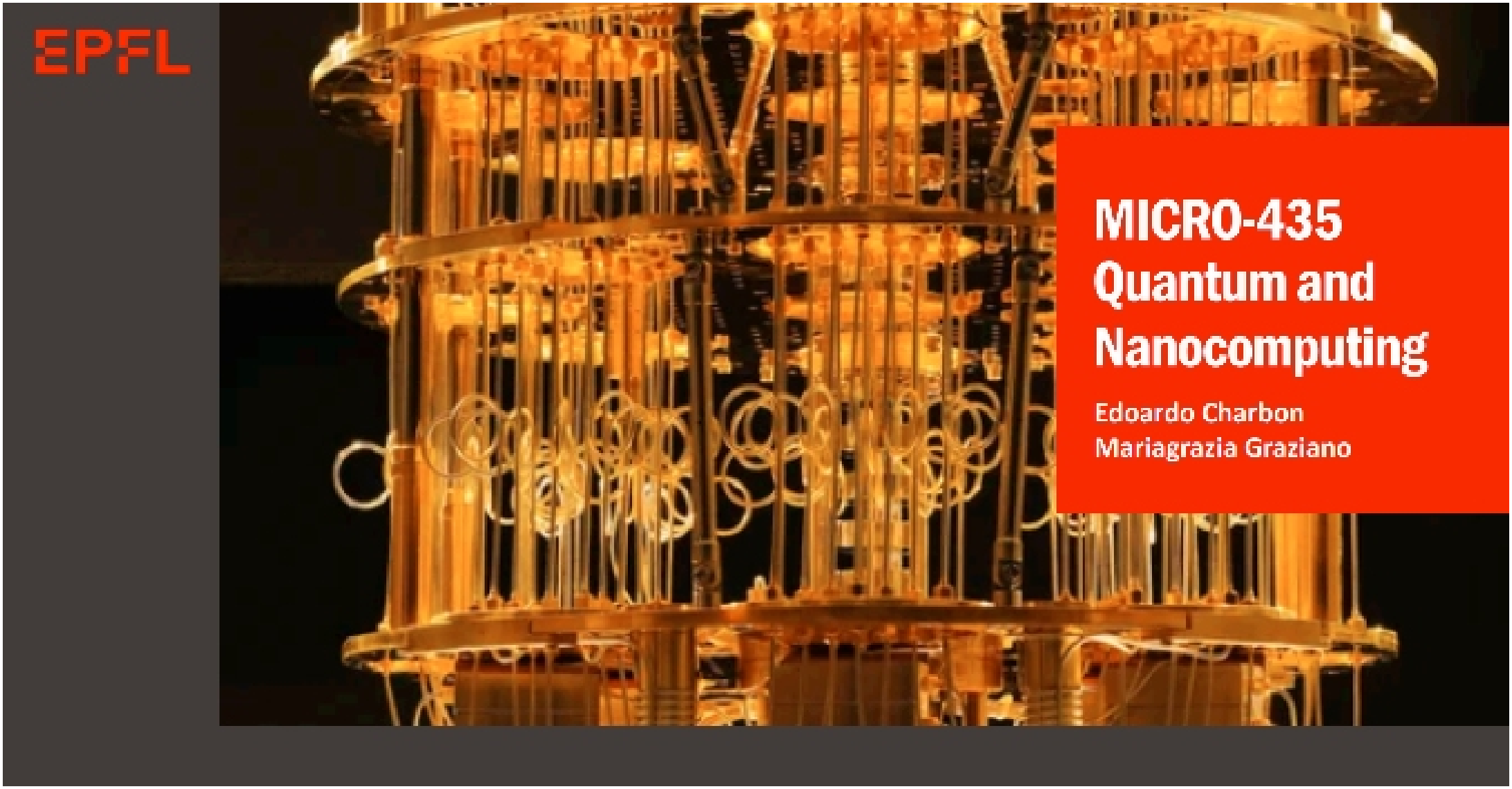


M.T. BEHAVIOR & CHARACTERISTIC

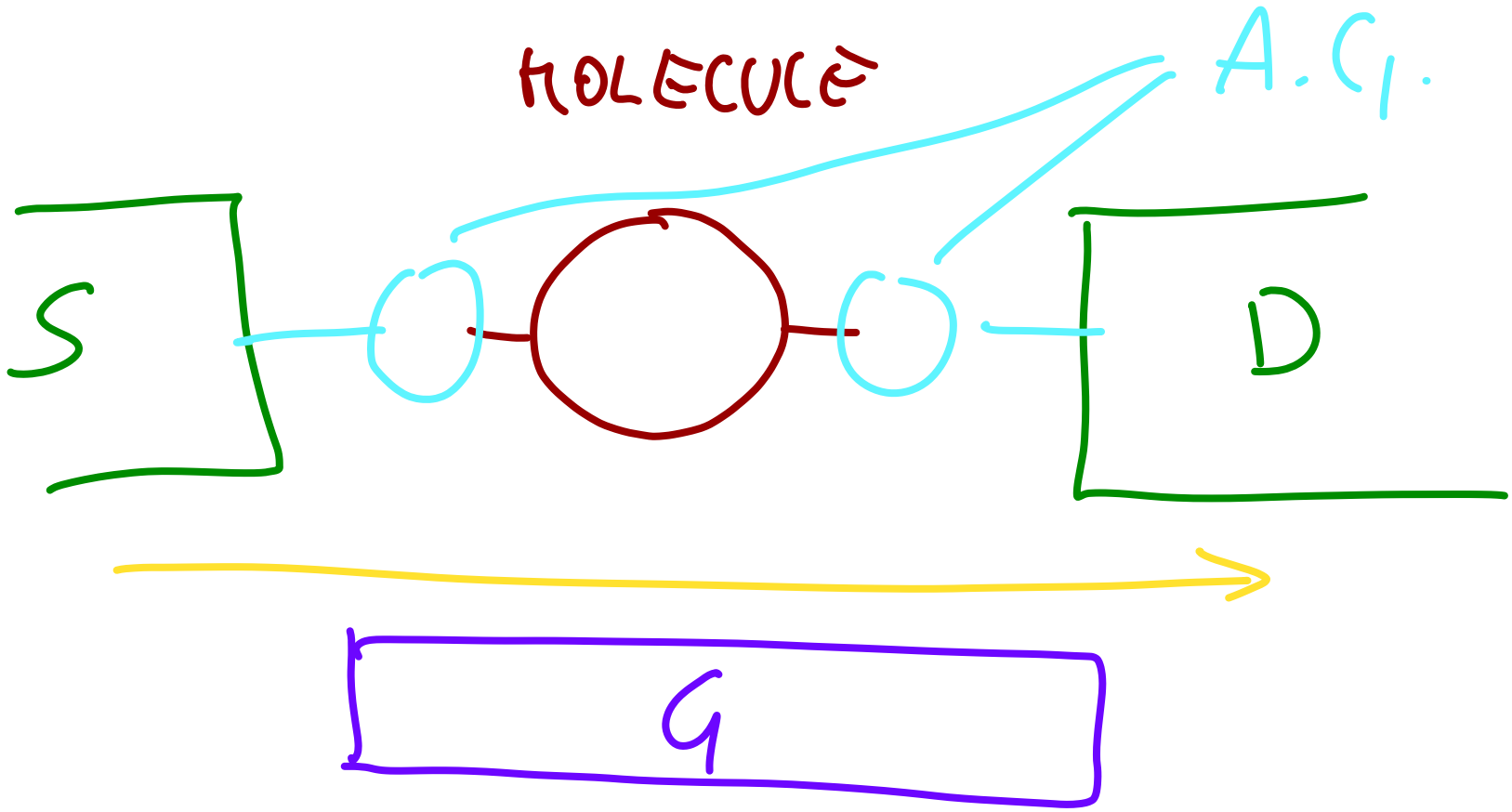
PART 1

H. T. MAIN PARAMETERS

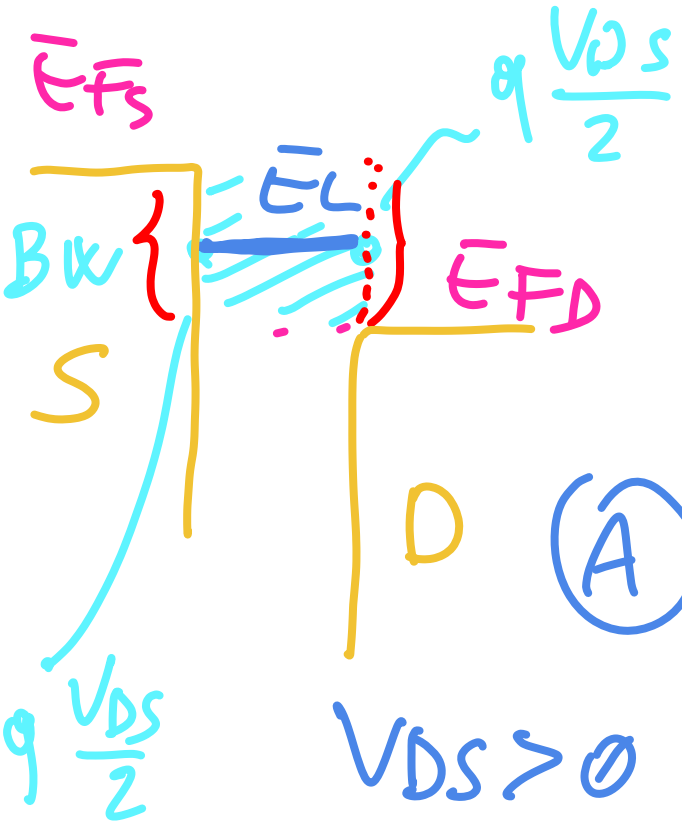
OBJECTIVES

a) RECALL HT CHARCTERISTICS

MOLECULAR TRANSISTOR
BEHAVIOR & APPLICATIONS



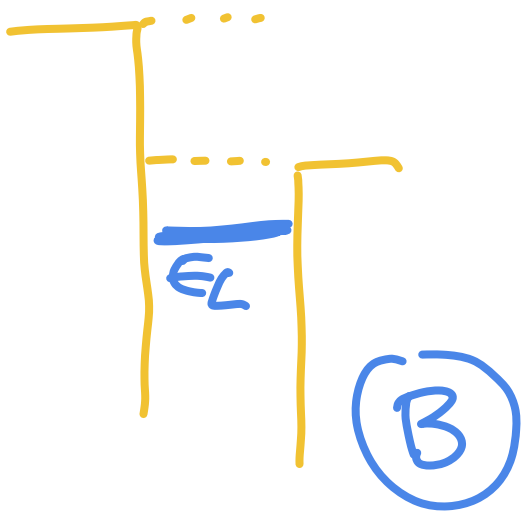
$$I_{DS} = \frac{2q}{\hbar} \cdot \underbrace{\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}}_{\text{COUPLING FACTOR}} \left[f(E_L, E_{FS}) - f(E_L, E_{FD}) \right]$$



A

$V_{DS} > 0$

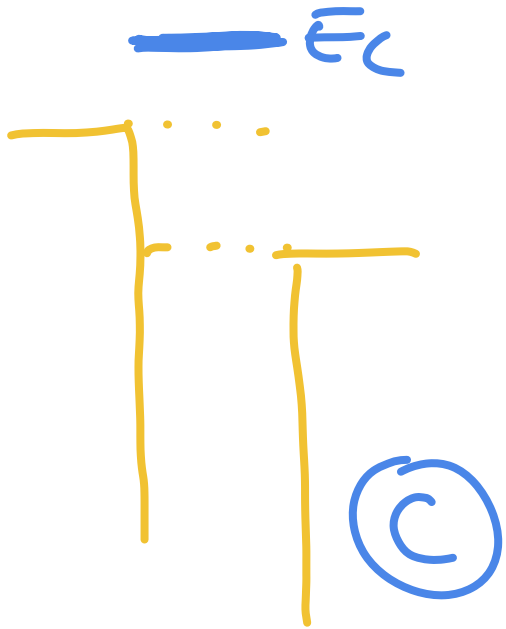
$I_{DS} > 0$



B

$V_{DS} > 0$

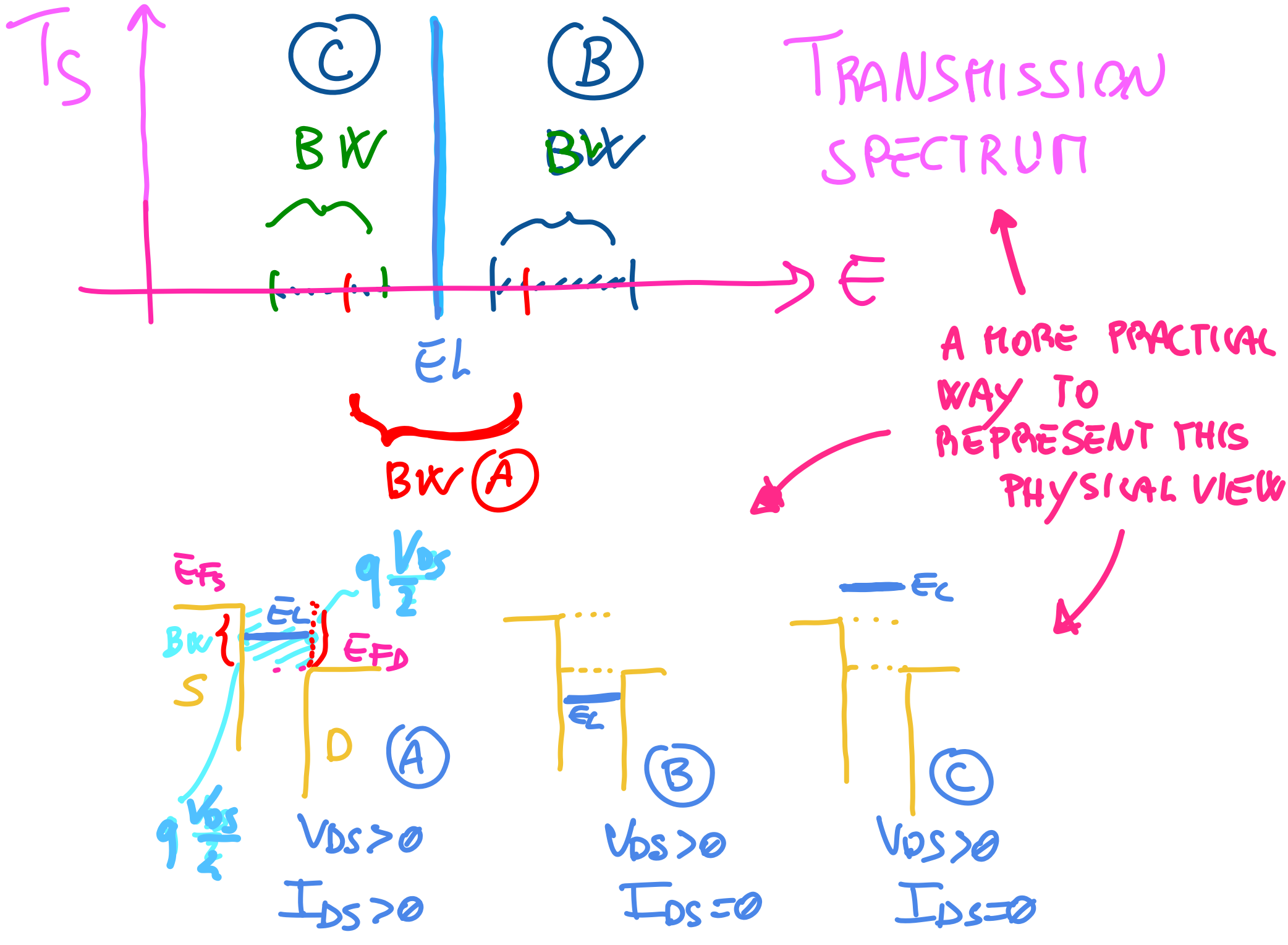
$I_{DS} = 0$

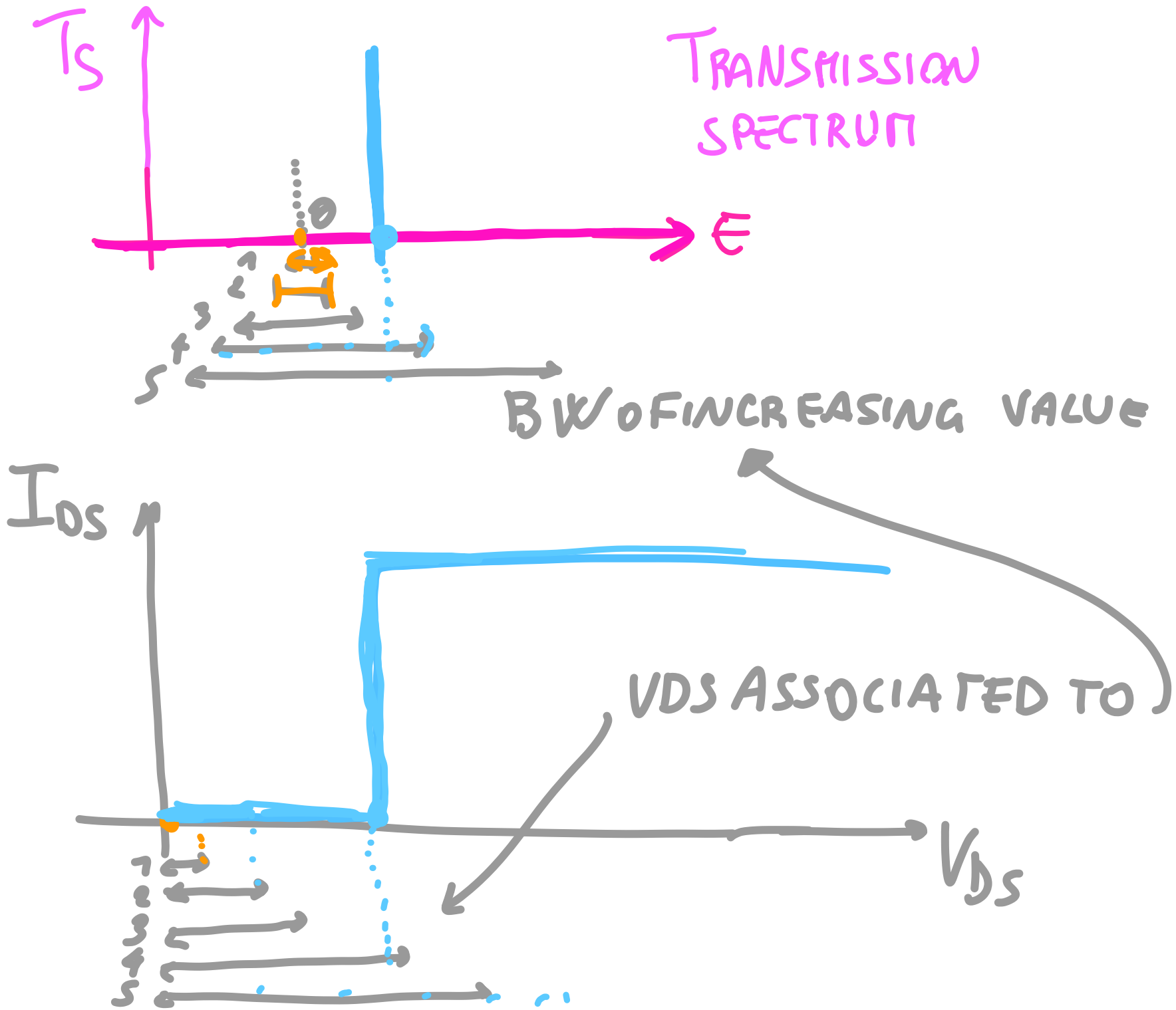


C

$V_{DS} > 0$

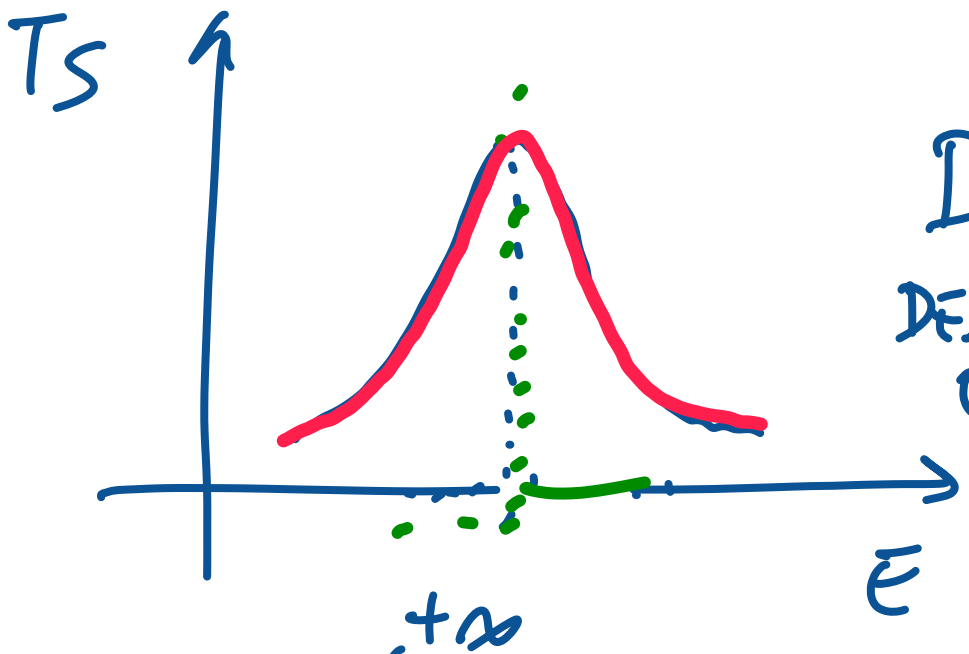
$I_{DS} = 0$


T_S
C
B
BW
BW
E_L
BW
A
E
TRANSMISSION SPECTRUM
A MORE PRACTICAL WAY TO REPRESENT THIS PHYSICAL VIEW
E_{FS}
E_L
$q\frac{V_{DS}}{2}$
BW
E_{FD}
S
D
A
$q\frac{V_{DS}}{2}$
$V_{DS}>0$
$I_{DS}>0$
E_L
B
$V_{DS}>0$
$I_{DS}=0$
E_L
C
$V_{DS}>0$
$I_{DS}=0$


Ts
TRANSMISSION SPECTRUM
0
E
BW OF INCREASING VALUE
IDS
VDS ASSOCIATED TO
VDS

IN CASE OF A MOLECULE → BROADENING

STRONG COUPLED DOT



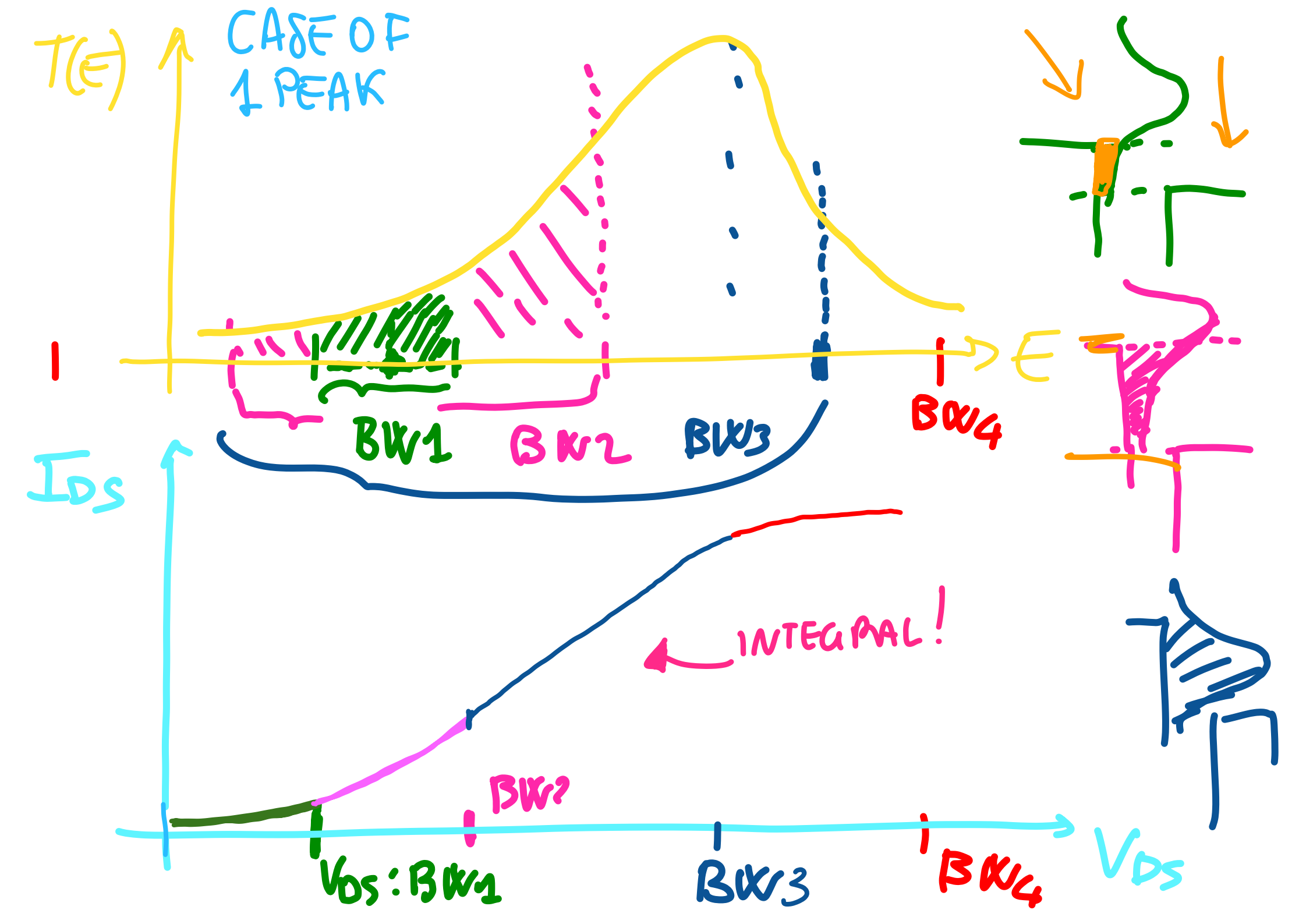
$$D(E) = \frac{\gamma/2\pi}{(E-E_L)^2 + \left(\frac{\gamma}{2}\right)^2}$$

DENSITY OF STATE

LORENTIAN DISTRIBUTION

$$I_{DS} = \frac{2q}{\hbar} \int_{-\infty}^{+\infty} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} D(E) \cdot \left[f(E, E_{FS}) - f(E, E_{FD}) \right]$$

TRANSMISSION SPECTRUM


T(E)
CASE OF
1 PEAK
BW1
BW2
BW3
BW4
E
IDS
INTEGRAL!
BW2
VDS : BW1
BW3
BW4
VDS

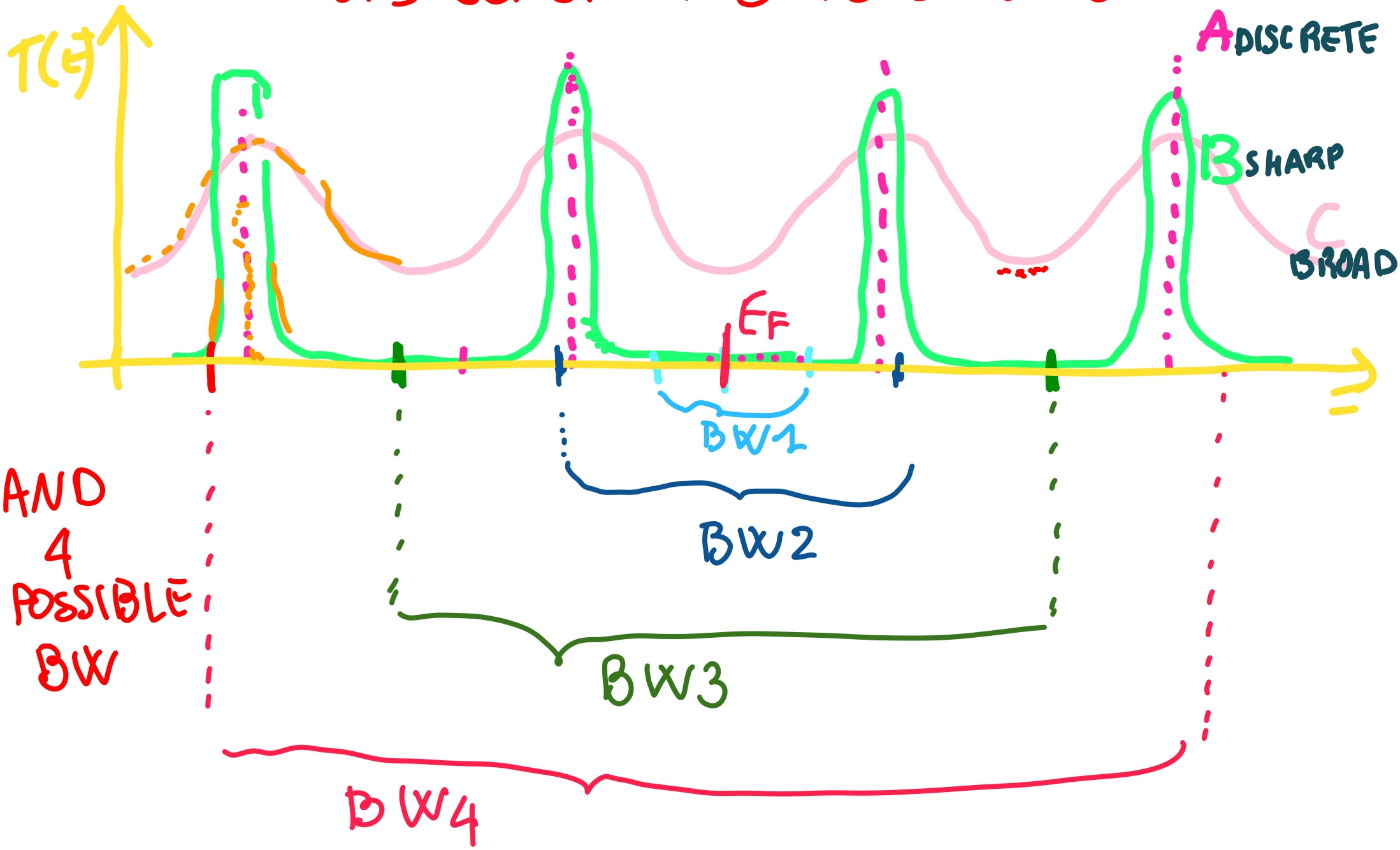
IN A REAL MOLECULE → MORE THAN ONE PEAK

COMPOSITION WITH BROADENING

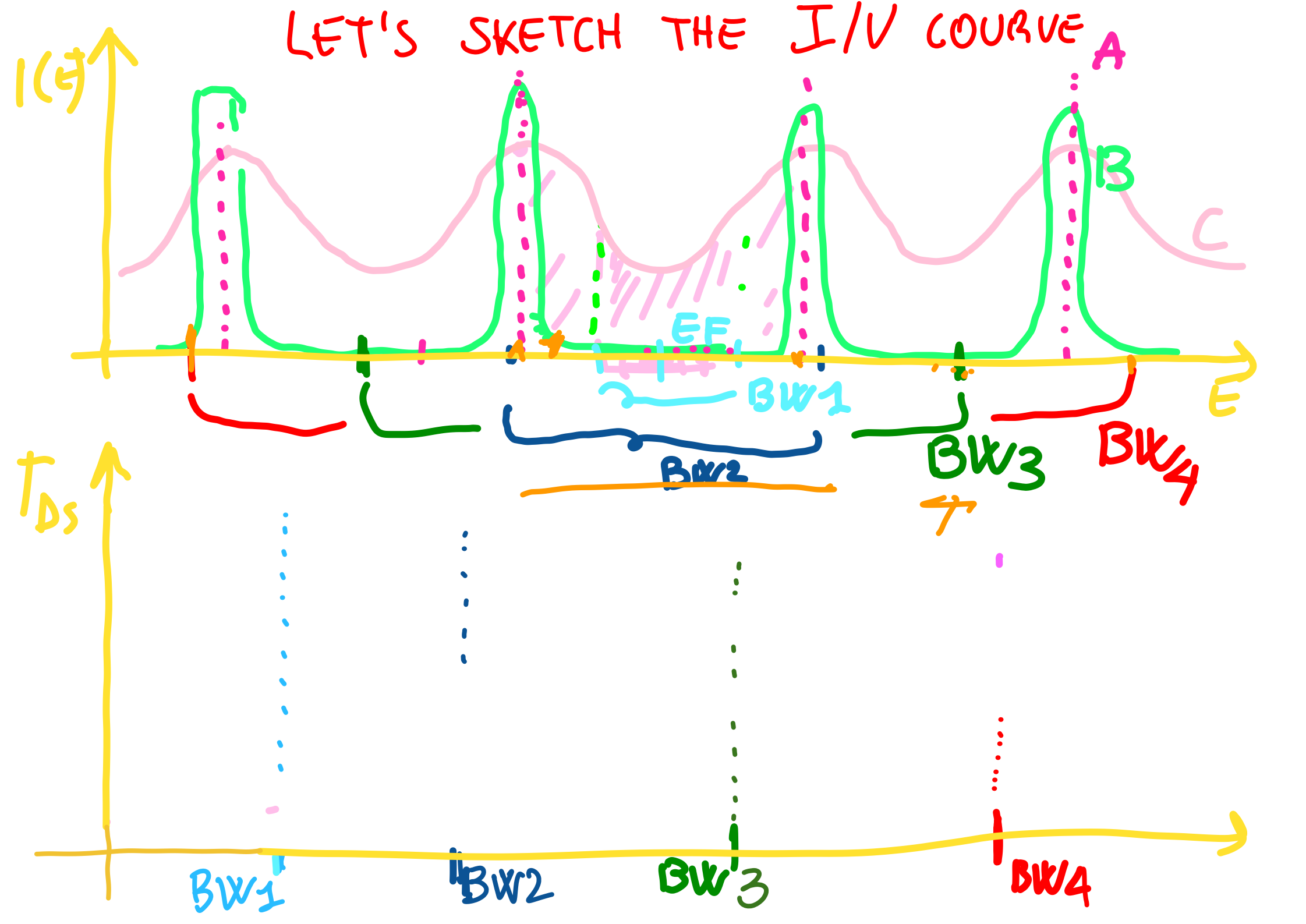
EXAMPLE

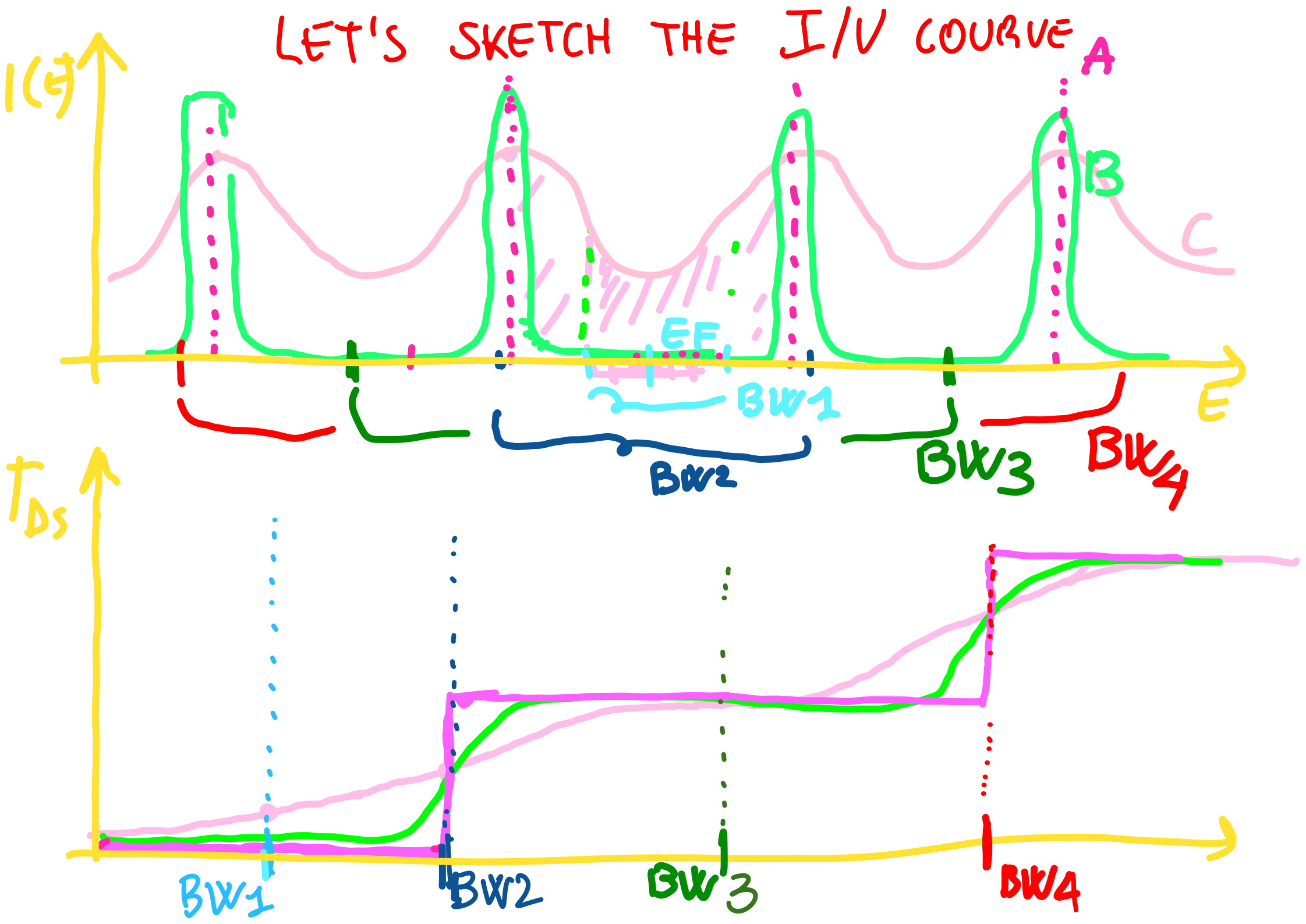
IN TERMS OF TRANSMISSION SPECTRUM

LET'S CONSIDER 3 POSSIBLE BROADENING

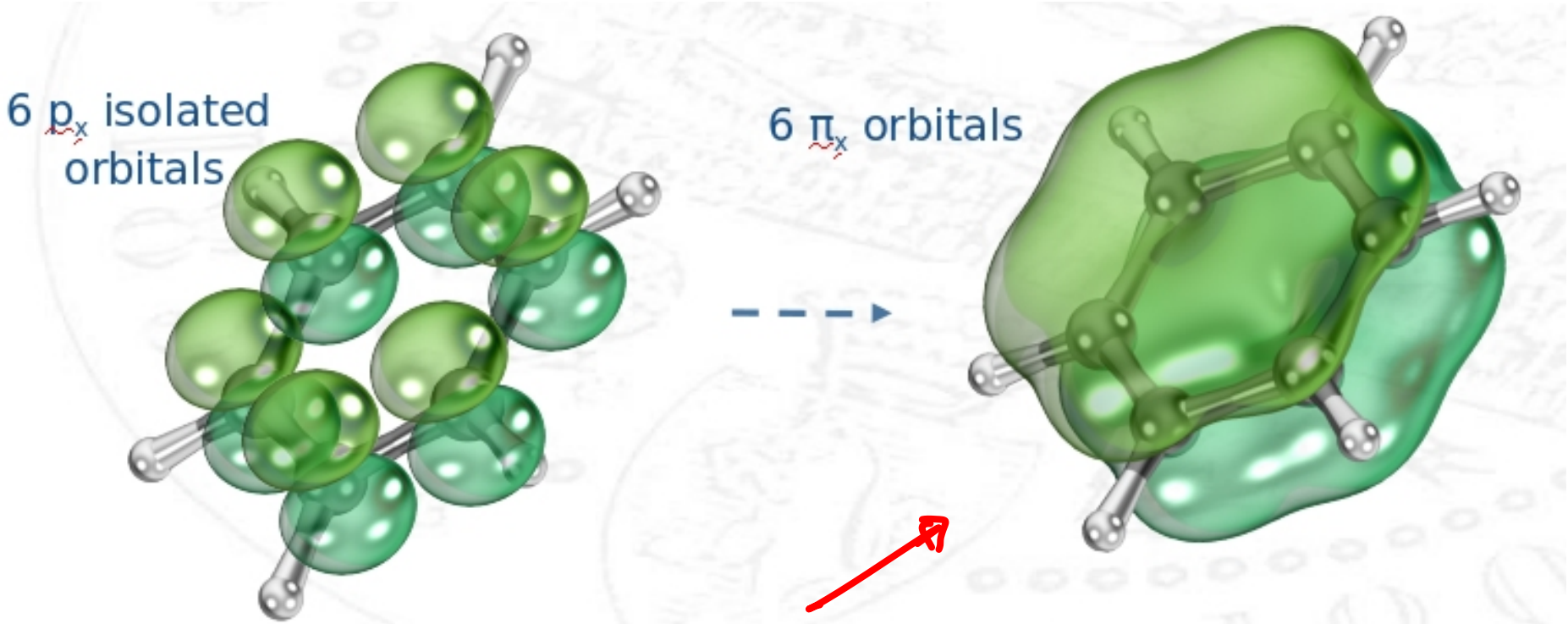


AND 4 POSSIBLE BW


LET'S SKETCH THE I/V COURVE
I(E)
A
B
C
EF
BW1
E
BW2
BW3
BW4
T_{DS}
BW1
BW2
BW3
BW4

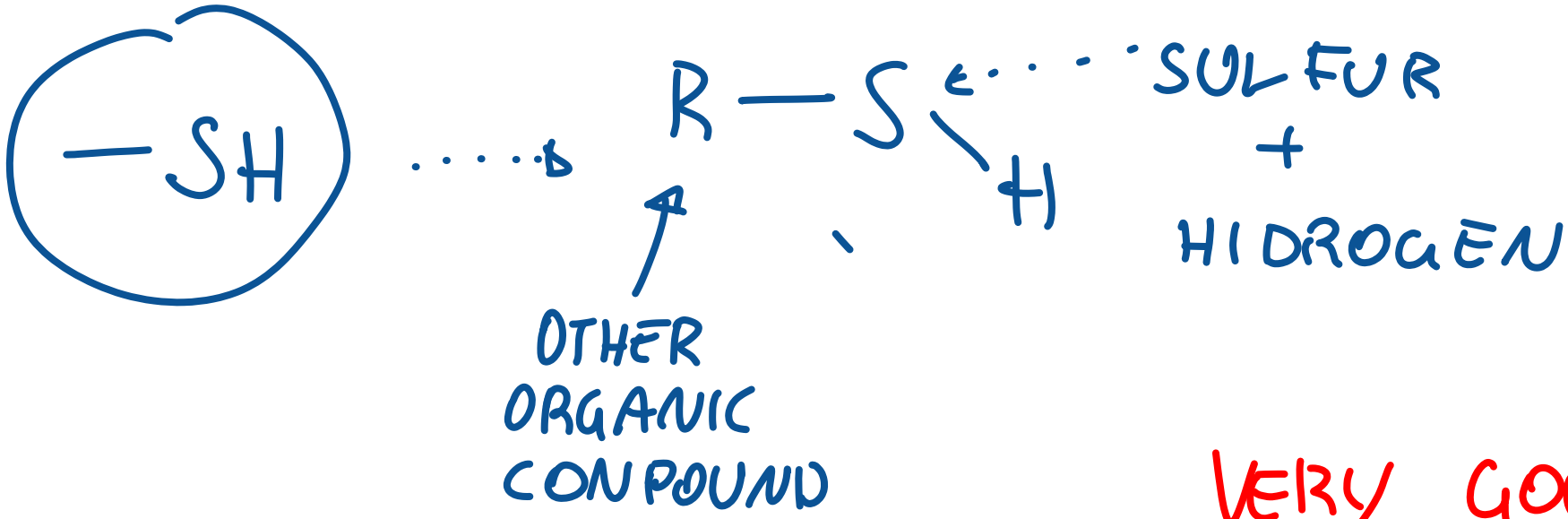

LET'S SKETCH THE I/V COURVE
I(E)
A
B
C
EF
BW1
E
BW2
BW3
BW4
I_{DS}
BW1
BW2
BW3
BW4

BENZENE → CONJUGATED MOLECULE

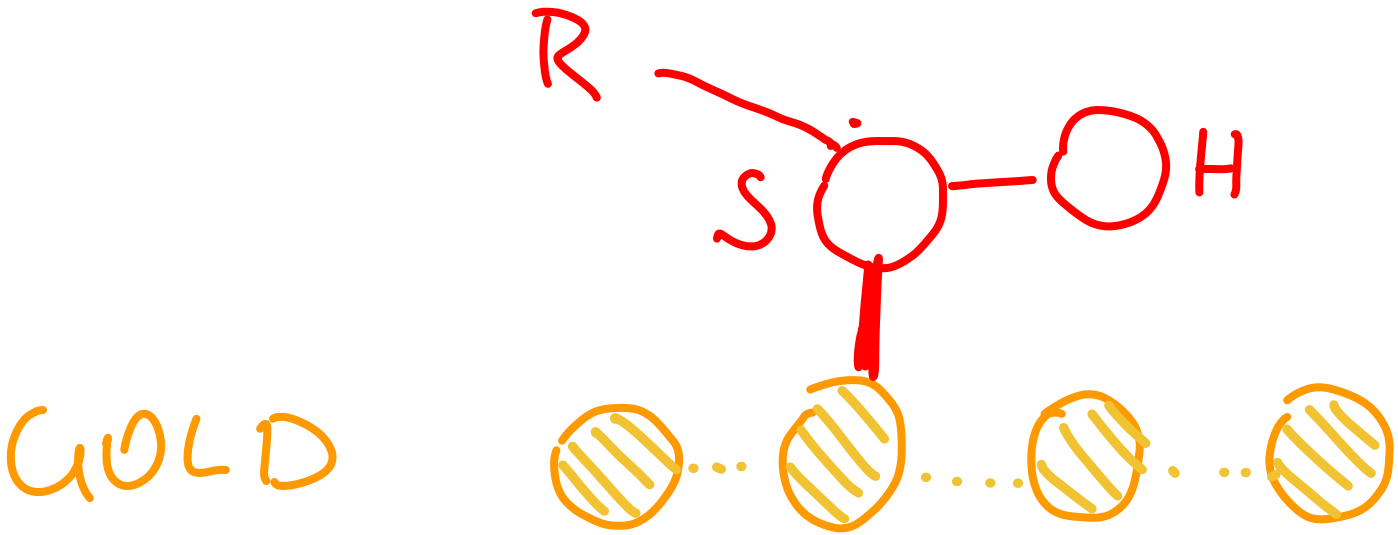


DELOCALIZATION OF ELECTRONS ACROSS ADJACENT ALIGNED π ORBITAL

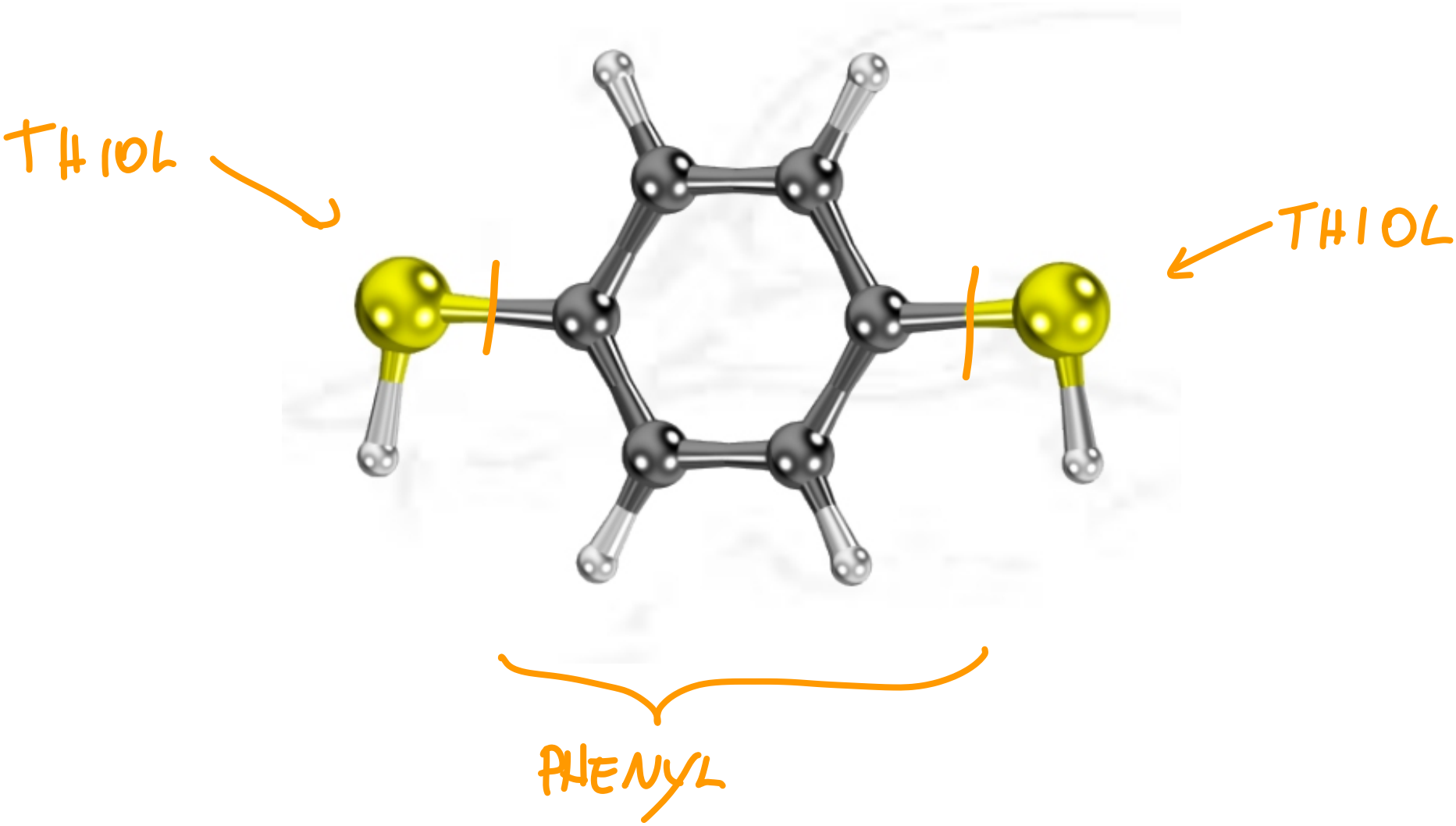
THIOL AS ANCHORING GROUP



VERY GOOD AFFINITY WITH GOLD

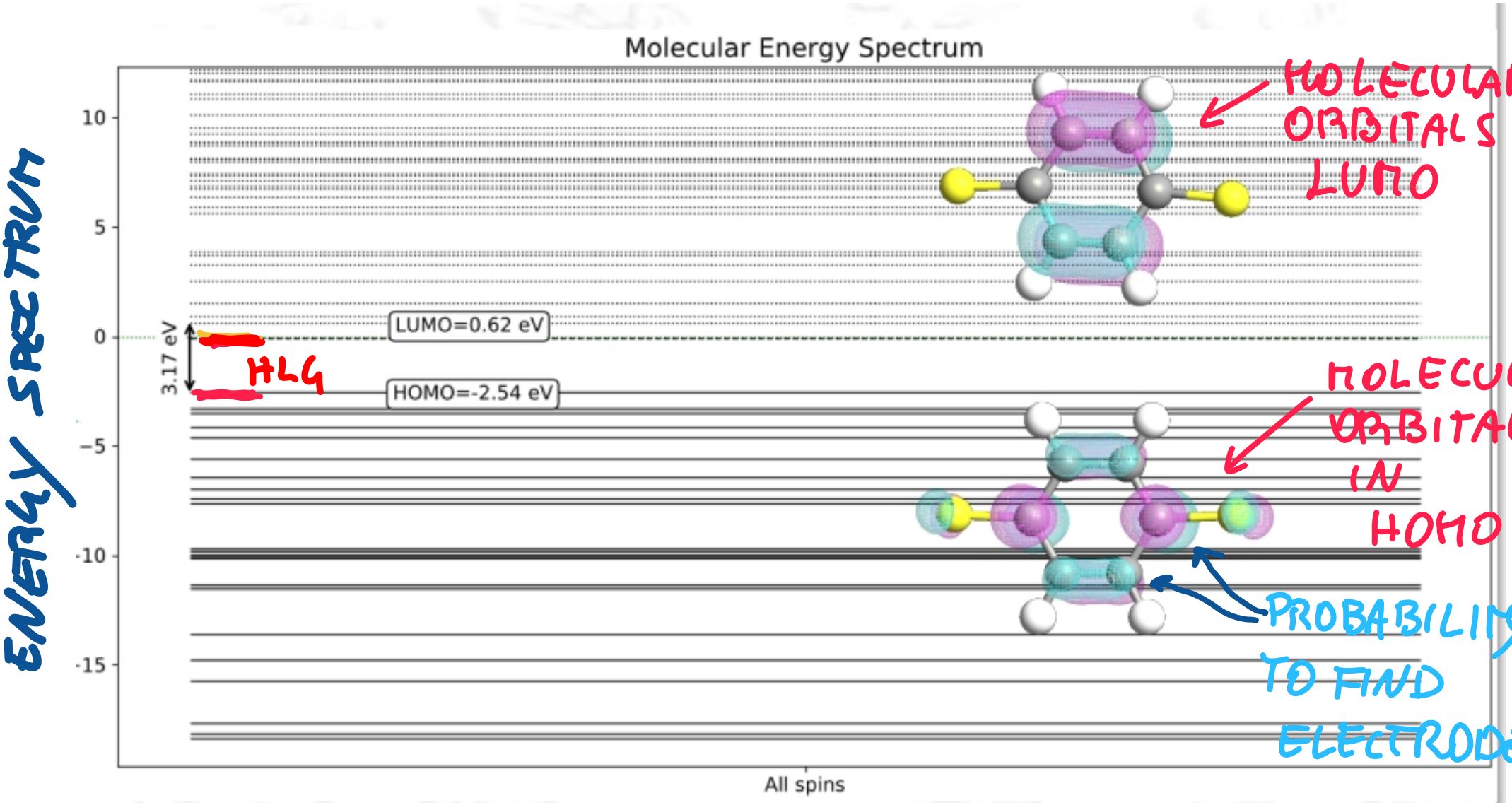


DITHIOL -BENZENE DTH



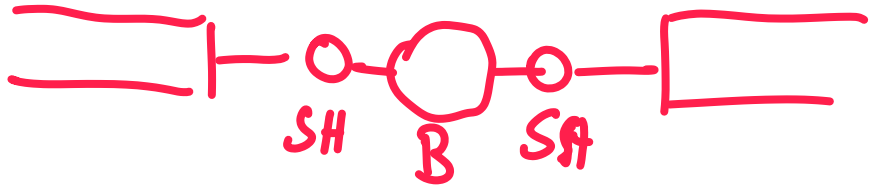
ISOLATED DTB - ANALYSIS

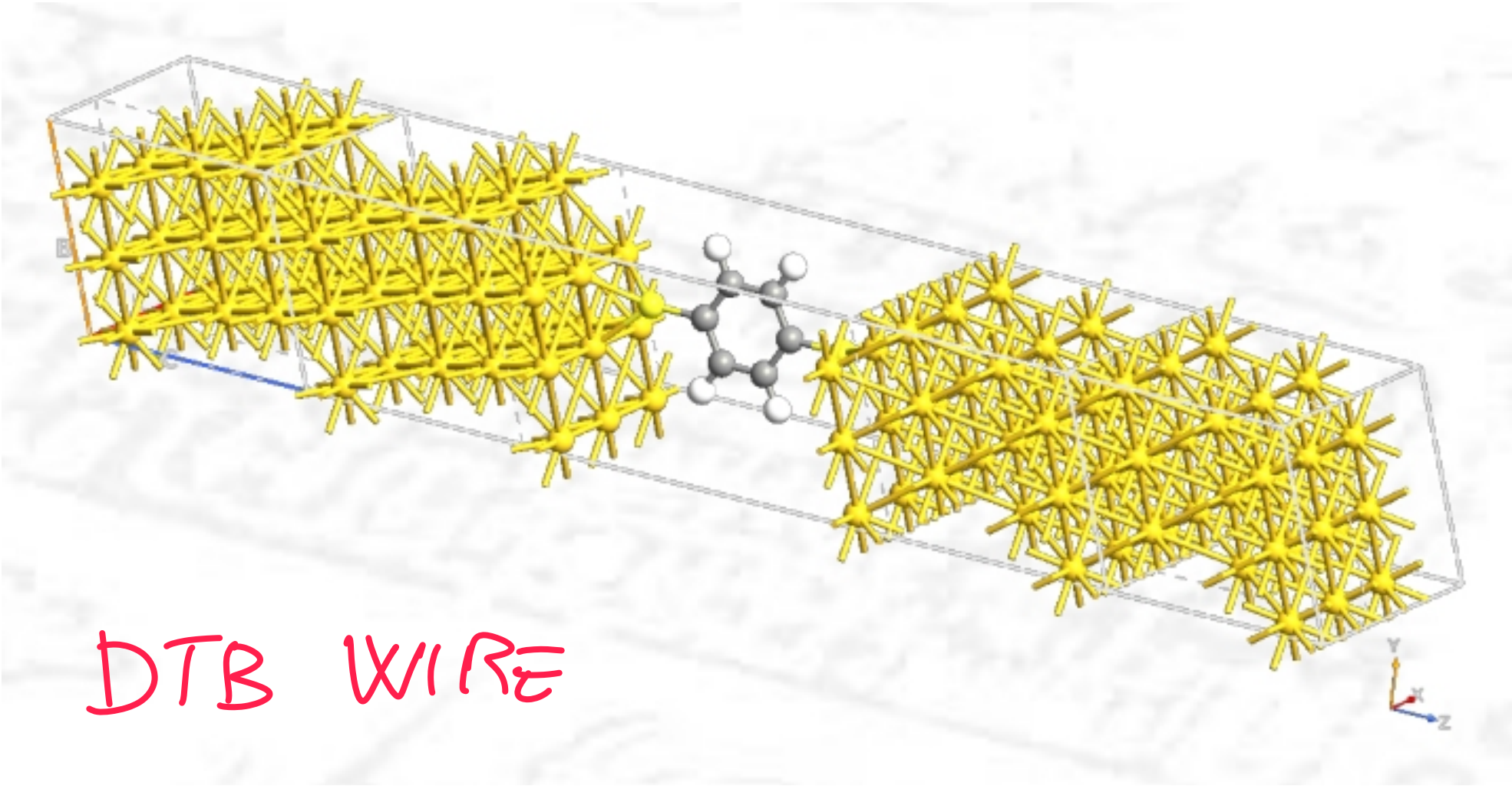
FERMI LEVEL EF = -5.56eV N. electrons 40



BASED ON QUANTUM ATK SIMULATION - CREDITS C.ELFISPANO

CONNECTION TO GOLD ELECTRODES



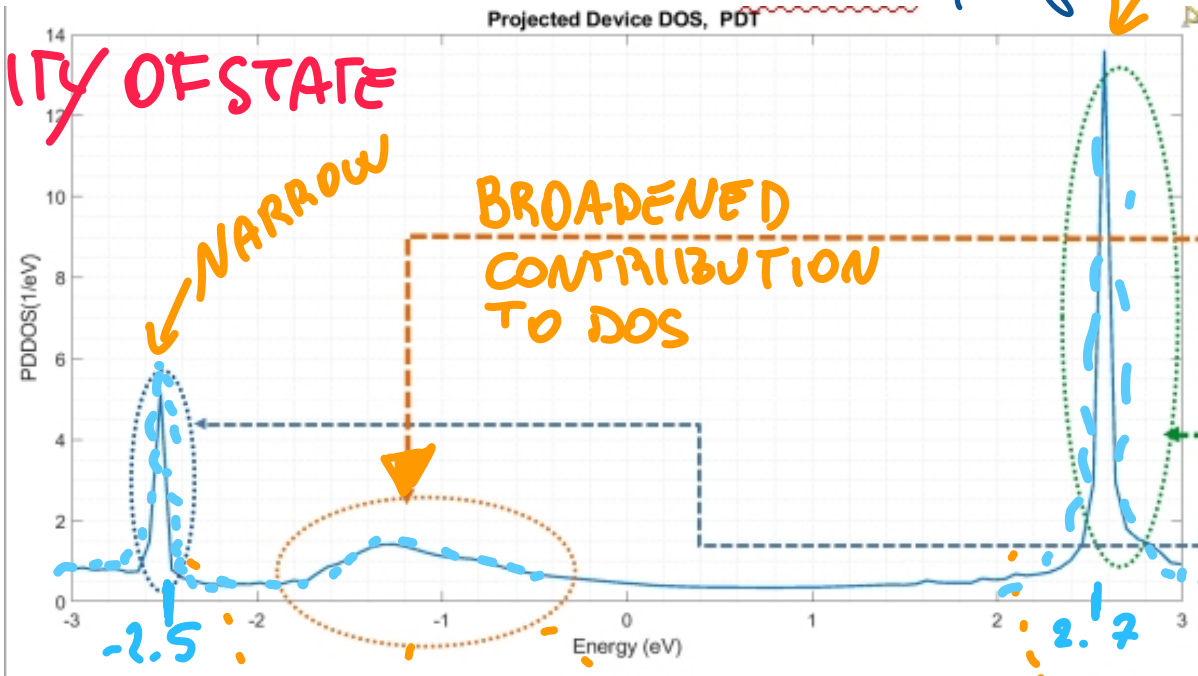


DTB WIRE

BDT WIRE

DENSITY OF STATE

HOLT A.G



not strong influence of electrodes

NARROW

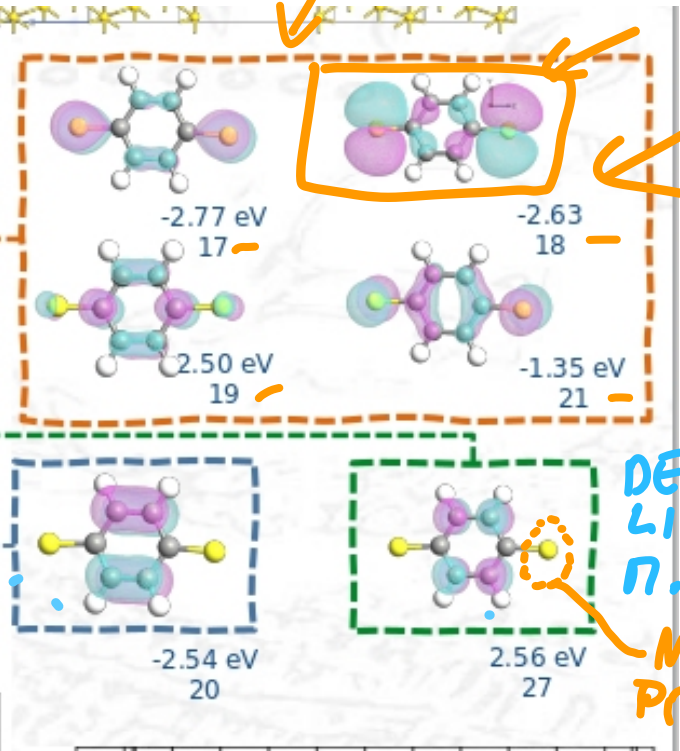
NARROW

BROADENED CONTRIBUTION TO DOS

-2.5

2.7

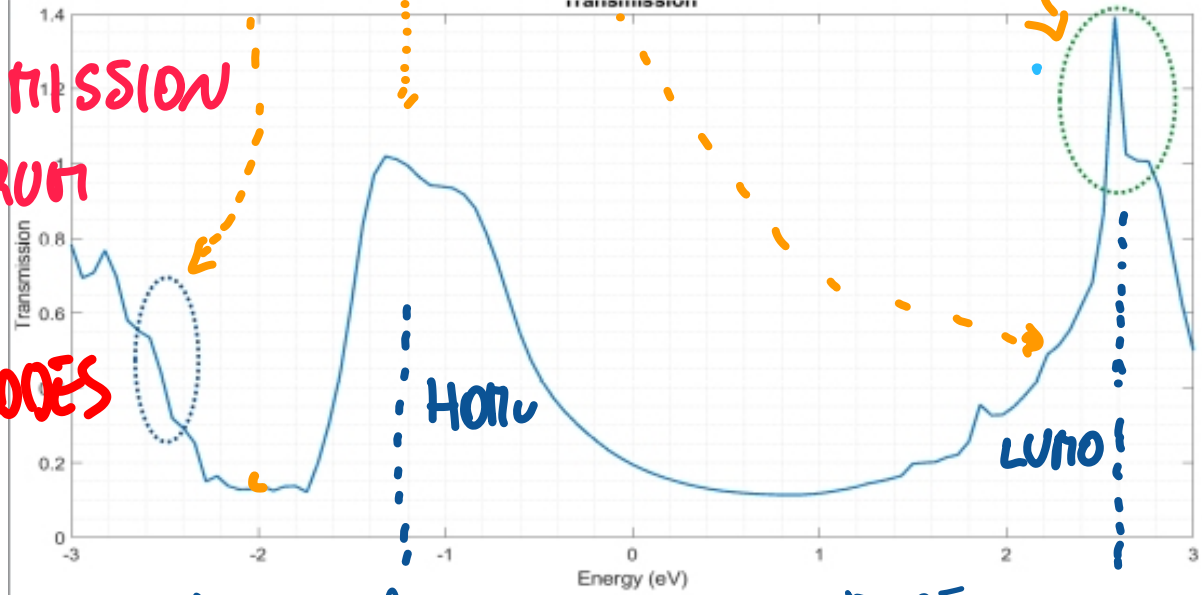
LARGER PEAKS

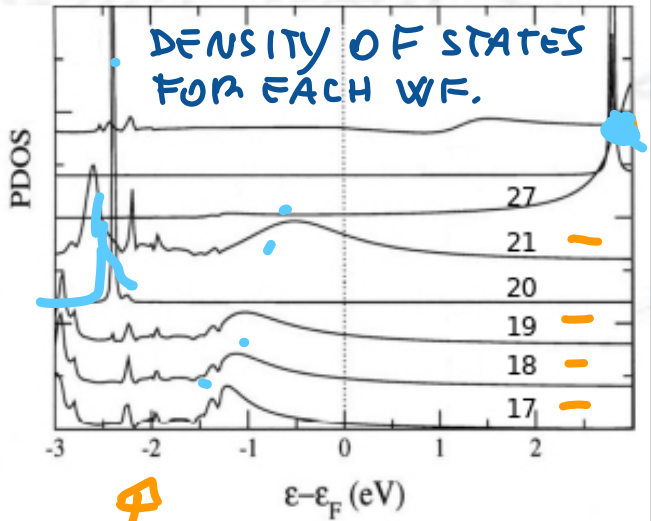


DELOCALIZE Π.O.

NO PROB TO FND EL.

TRANSMISSION SPECTRUM WITH ELECTRODES





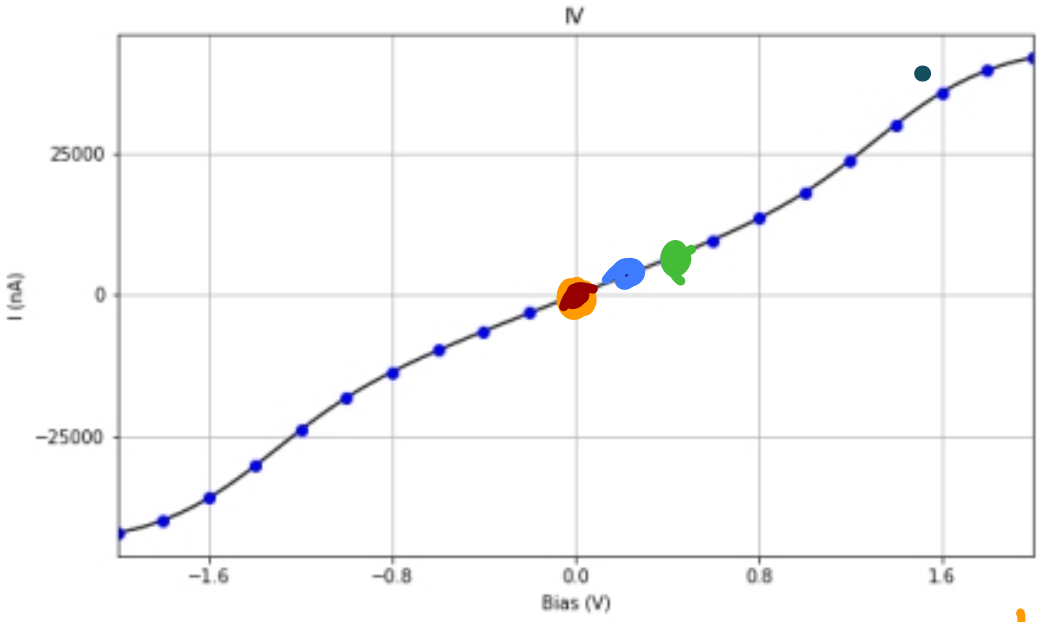
quantum numbers

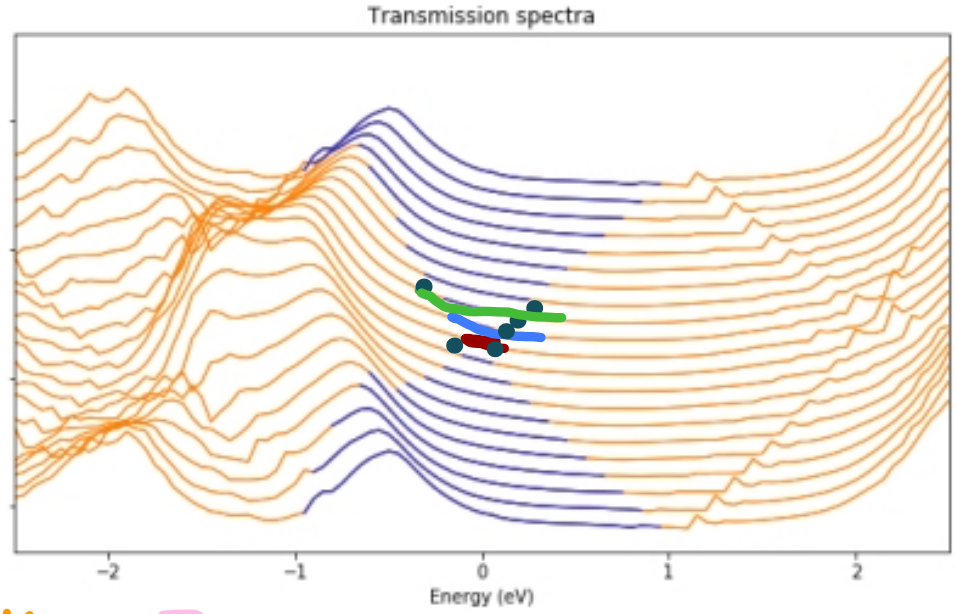
strong influence of electrodes → MORE BRADENED → LARGER PEAKS

I/V CURVE

↓

TS for different applied V





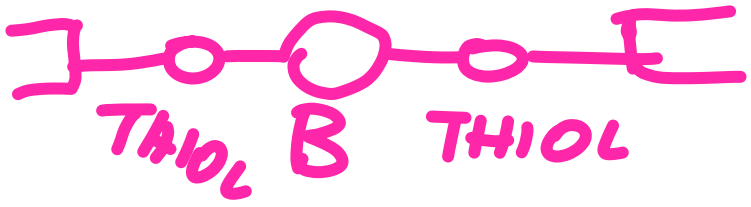
−2 V +2V

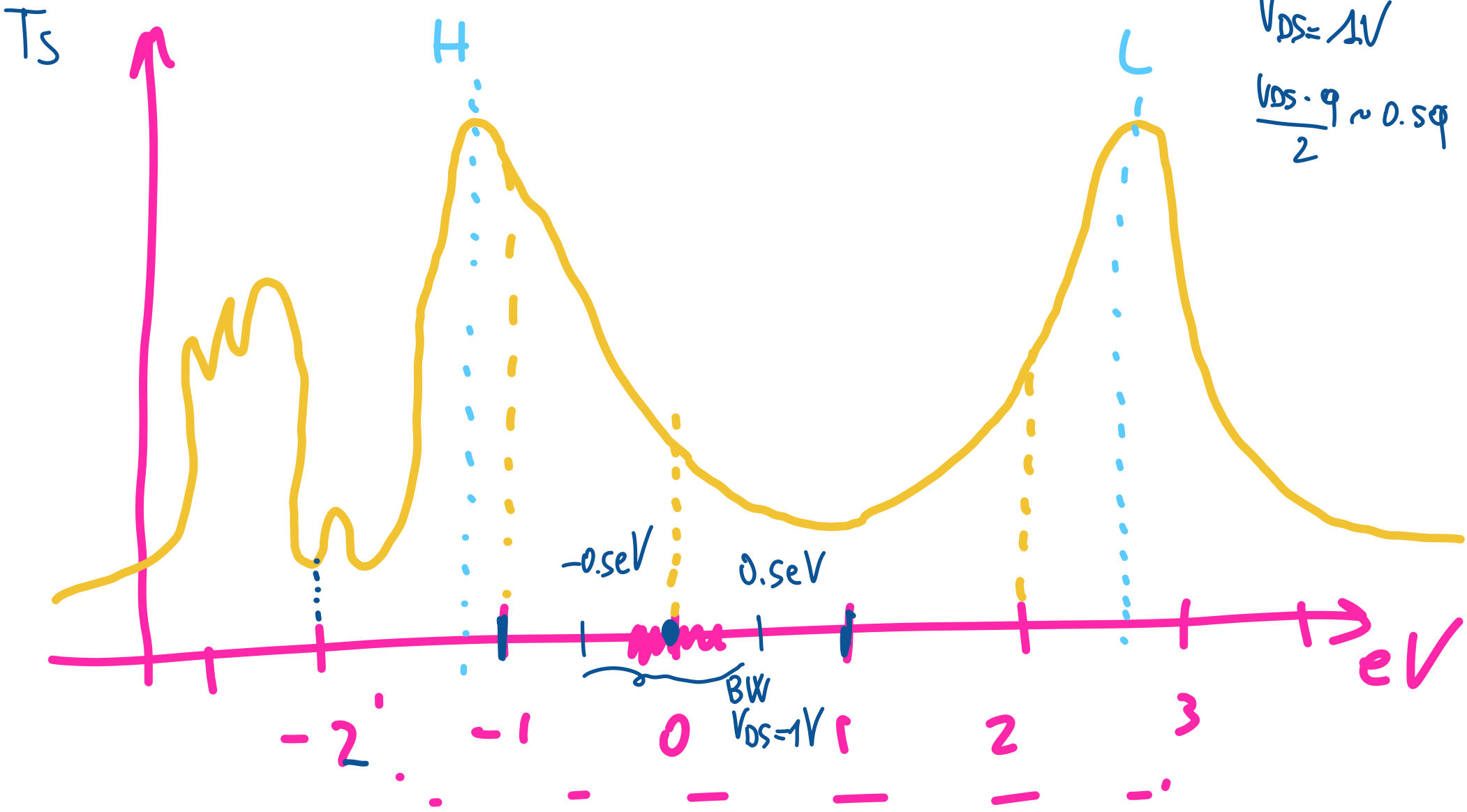
NOTICE THAT ∀ APPLIED V and the ∀ BW THE TS CHANGES.... WHY ???

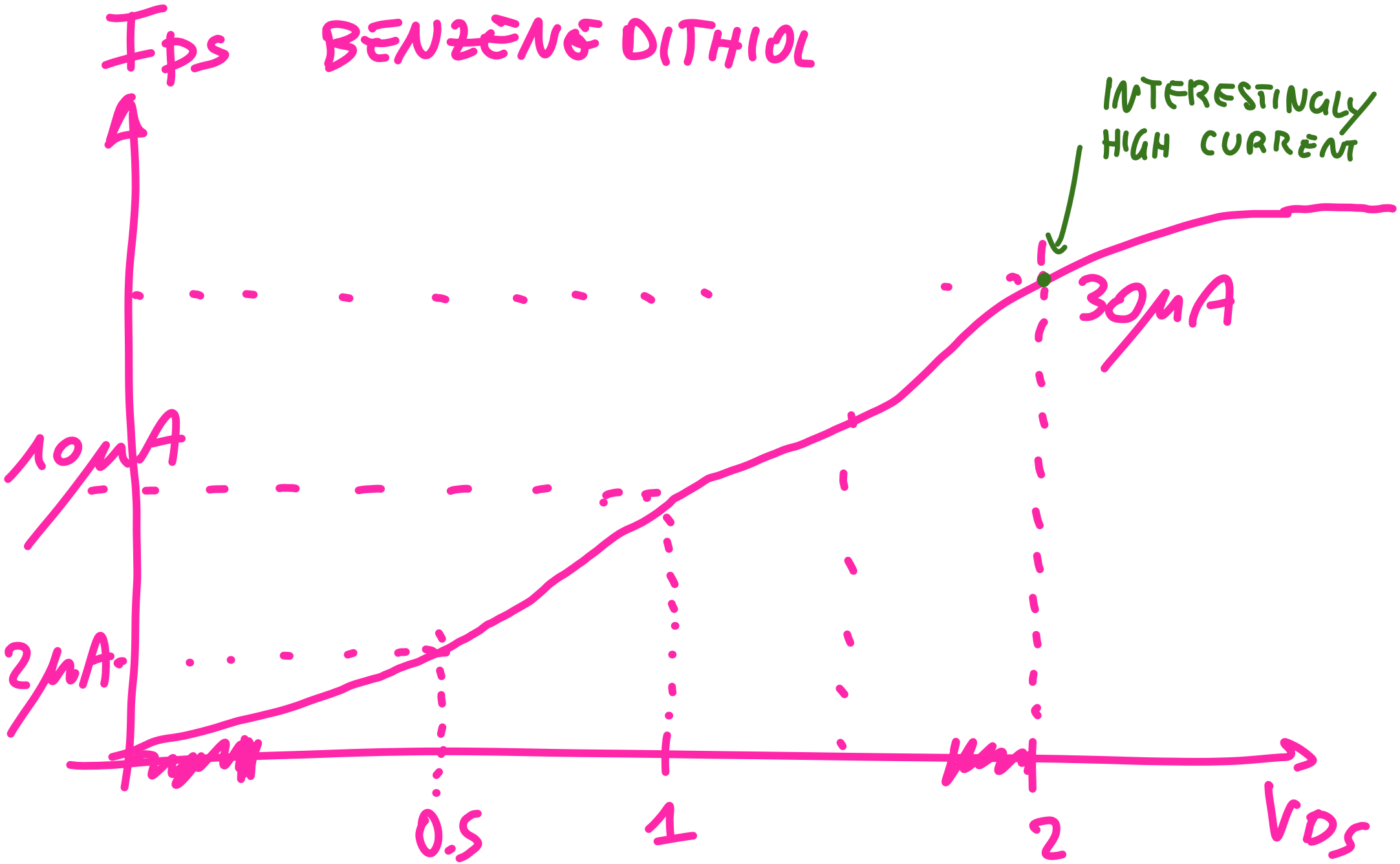
BLUE ZONES CORRESPOND TO B.WINDOW

MORE SIMPLY

BDT






I_{DS}
BENZENE DITHIOL
INTERESTINGLY HIGH CURRENT
30μA
10μA
2μA
0.5
1
2
V_{DS}