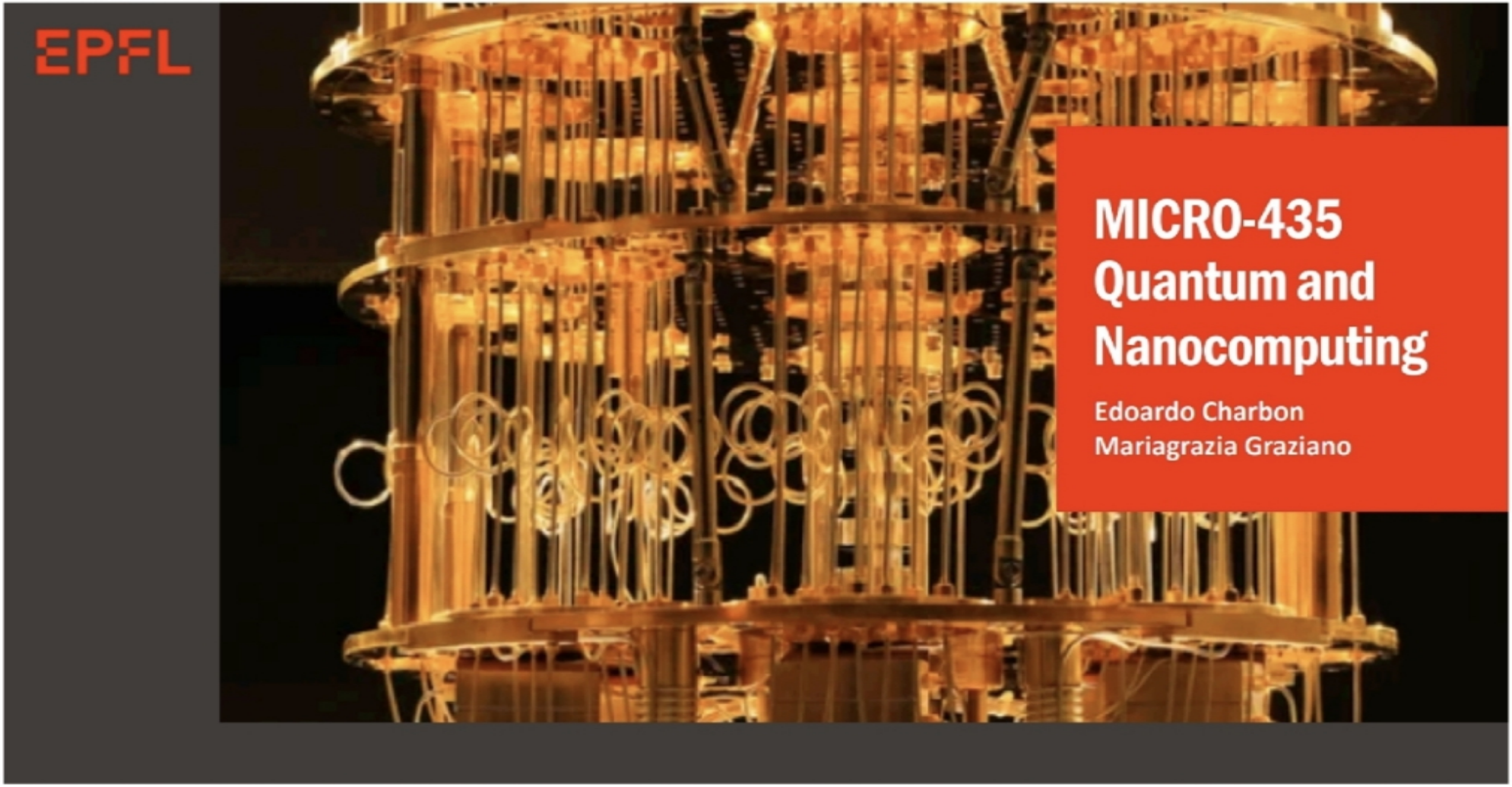


MT - SCF LOOP

& EEBESD MT SIMULATOR

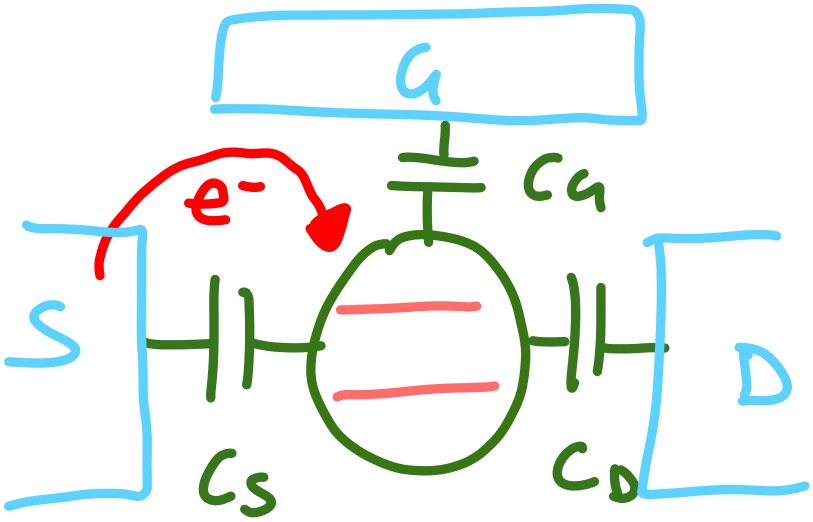
OBJECTIVES

a) SCF LOOP

b) SIMPLE CIRCUITS BASED ON MT

a) SCF LOOP

CAPACITIVE MODEL OF QDOT



$$C_{ES} = C_S + C_D + C_G + C_{BG}$$

$$U_{DOT} = -qV_{DS}\frac{C_D}{C_{ES}} - qV_{GS}\cdot\frac{C_G}{C_{ES}} + \frac{q^2}{E_S}\cdot(N - N_0)$$

CHARGING EFFECT

ACTUAL N° OF e^- IN THE DOT

N° of e^- @ Eq.

$$U \begin{cases} U_{VDS} = -q \dfrac{C_D}{C_{ES}} V_{DS} \\ U_{VGS} = -q \dfrac{C_G}{C_{ES}} V_{GS} \\ U_{C.E.} = \dfrac{q^2}{C_{ES}} \cdot \Delta N \end{cases}$$

$$\Delta N = N - N_0 \leftarrow \text{No el. @ EQ.}$$

$V_{GS} > 0$ U SHIFTS LOWER ENERGY

$V_{GS} < 0$ U SHIFTS HIGHER ENERGY

$+ V_{BG}$ IF PRESENT!

U_{SCF} SELF CONSISTING FIELD

$$U_{SCF} = U_0 (N - N_0)$$

N el. @ EQ.

actual N of el. involved in conduction

$$N = \int_{-\infty}^{+\infty} D(E - U_{SCF}) \cdot \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \left[f(E - E_{FS}) - f(E - E_{FD}) \right]$$

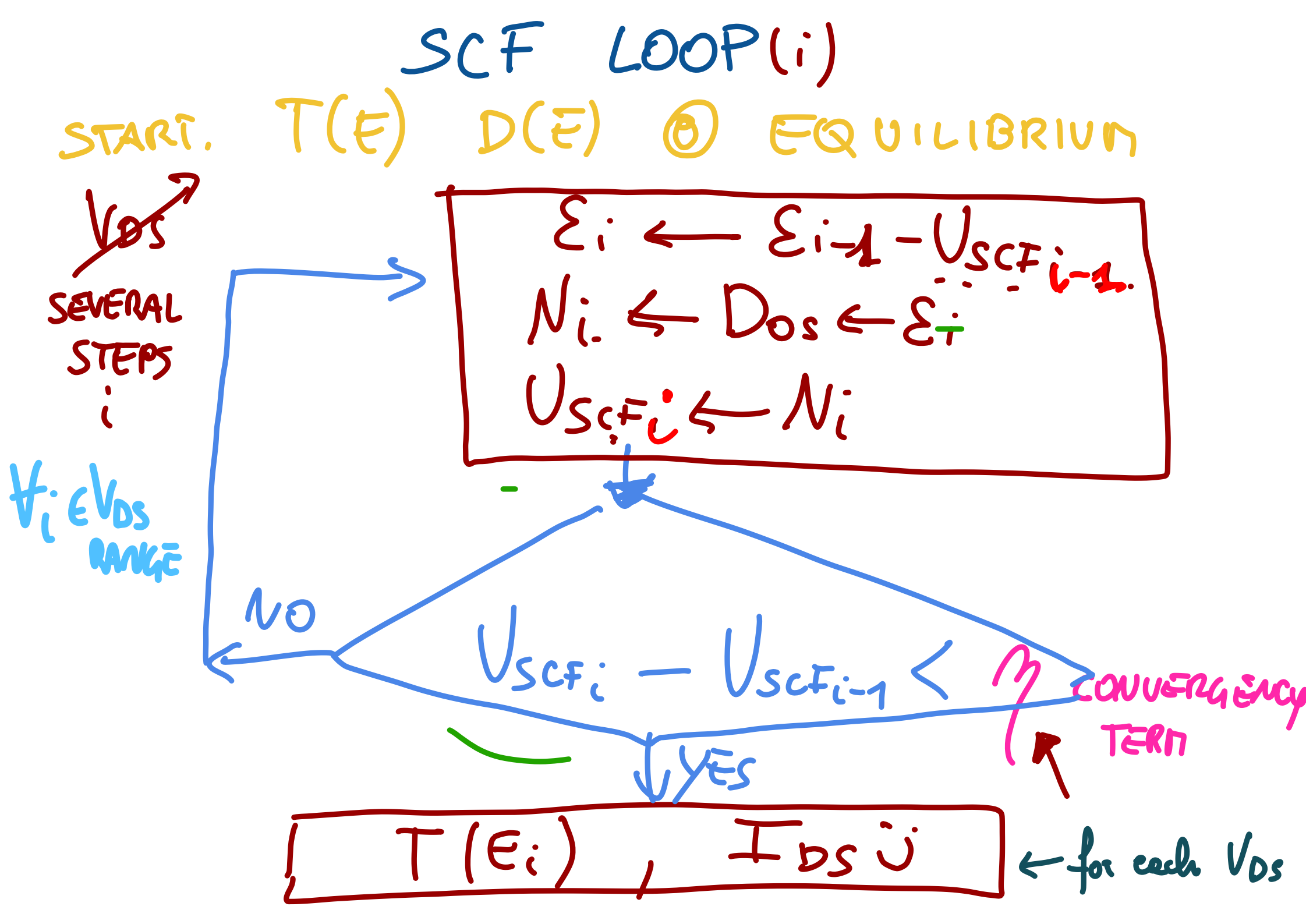
DOS of SHIFTED EN.

$U_{SCF} \leftarrow N$

$N \leftarrow U_{SCF}$

LOOP

HOW CAN WE FIND THE ACTUAL N FOR A CERTAIN CONDITION?

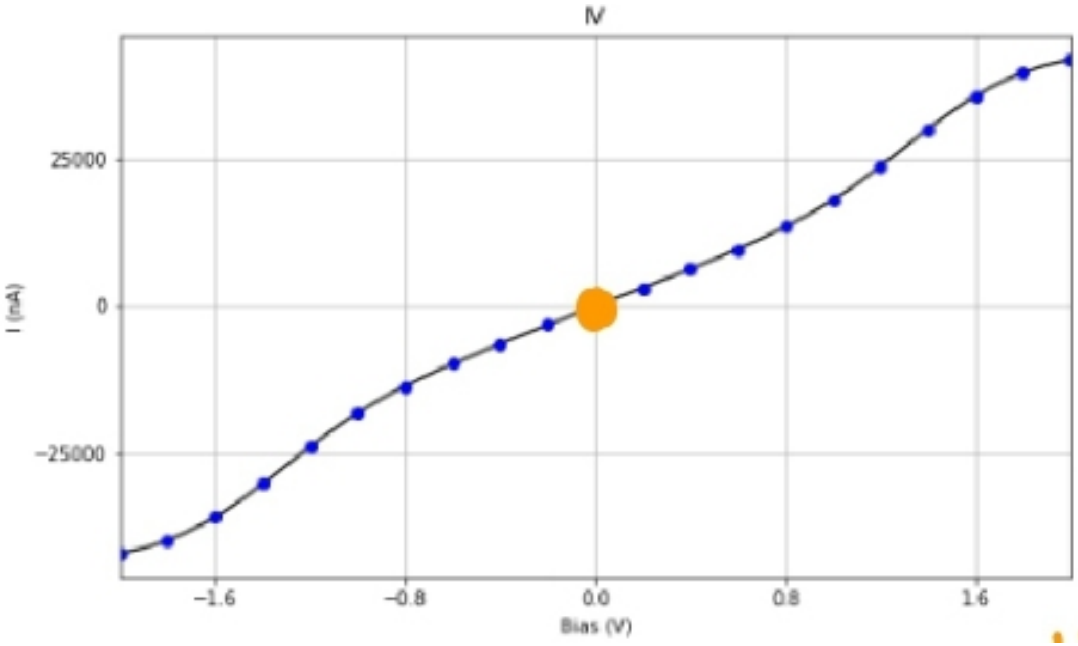

SCF LOOP (i)
START. T(E) D(E) @ EQUILIBRIUM
VDS
SEVERAL STEPS i
$\forall_i \in V_{DS}$ RANGE
$\varepsilon_i \leftarrow \varepsilon_{i-1} - U_{SCF\,i-1}$
$N_i \leftarrow DOS \leftarrow \varepsilon_i$
$U_{SCF\,i} \leftarrow N_i$
NO
$U_{SCF\,i} - U_{SCF\,i-1} < \eta$
CONVERGENCY TERM
YES
$T(E_i)$, I_{DS} ...
← for each V_{DS}

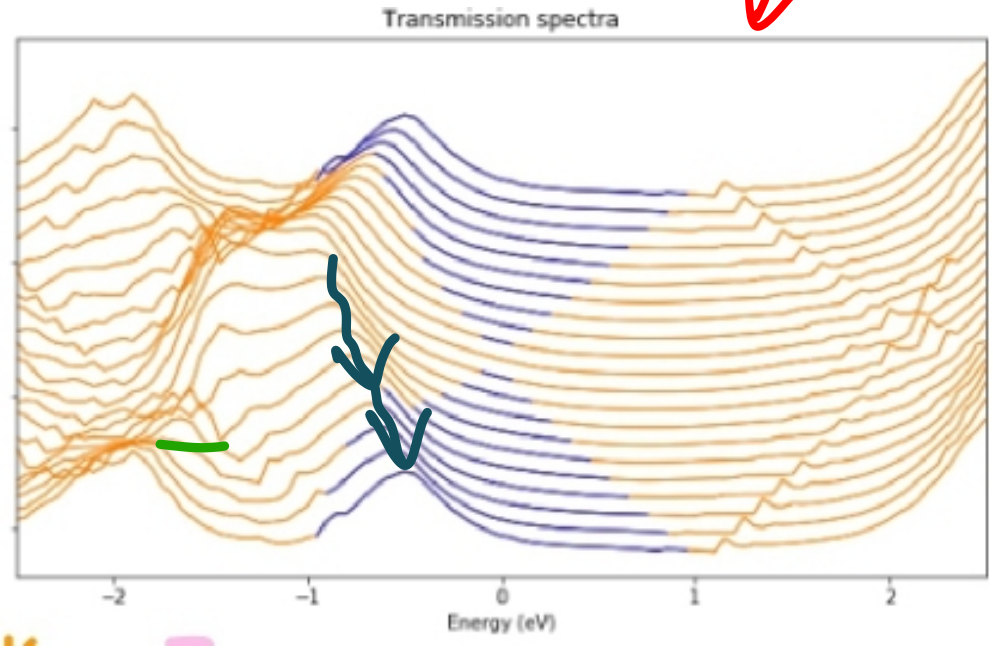
PROBLEM! N ← D ← PEAKS!

100%

HOW DOS CHANGES W.R.T. ⓪ EQUILIBRIUM

HOW TO EVALUATE?

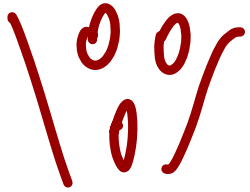




PROBLEM!

N ← D ← PEAKS!

HOW DOS CHANGES W.R.T. ⓪ EQUILIBRIUM



HOW TO EVALUATE?

QUANTUM-ATK

AB INITIO SIMULATION

- PRECISE
- CPU CONSUMING

EEBESD

ESTIMATE

HOW PEAKS CHANGE WHEN V_{DS} (V_{GS}) CHANGE

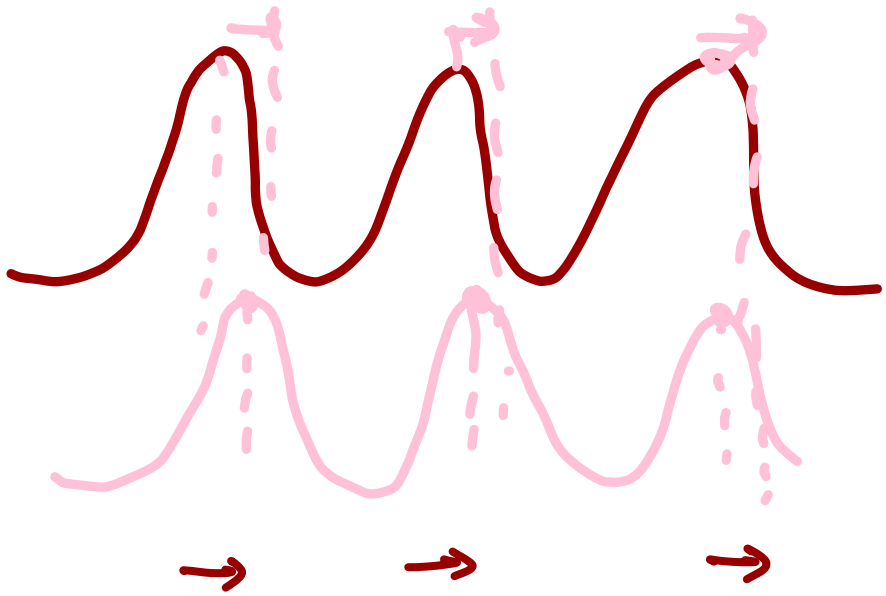
BASED ON { AB INITIO OR EXP.

EEBESD - SOLVES SCF LOOP

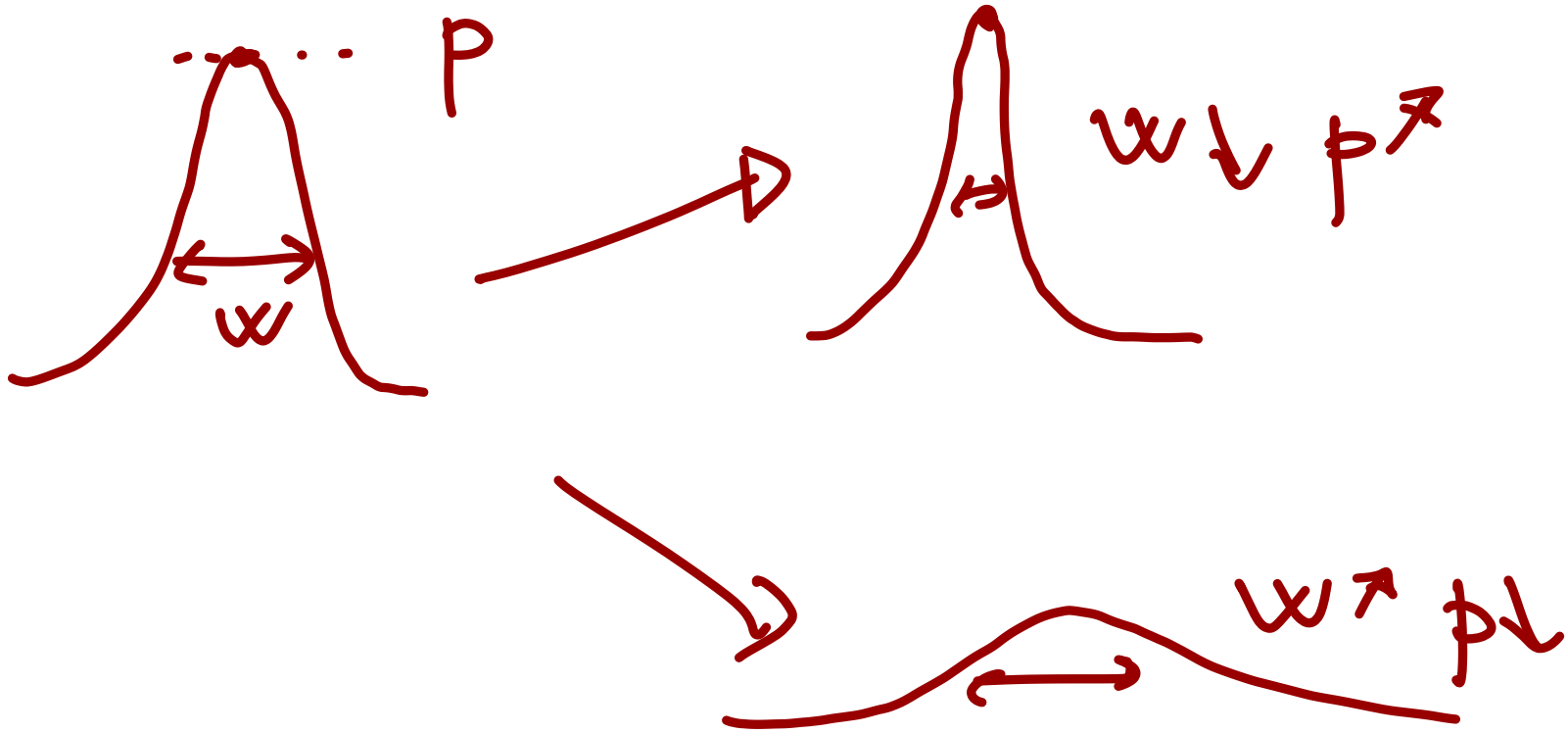
- ESTIMATES DOS
- BASED ON A BUNCH OF PRELIMINARY AB-INITIO SIN

ASSUMPTIONS

(1) WHEN V_{DS} APPLIED PEAKS SHIFT RIGIDLY



(2)

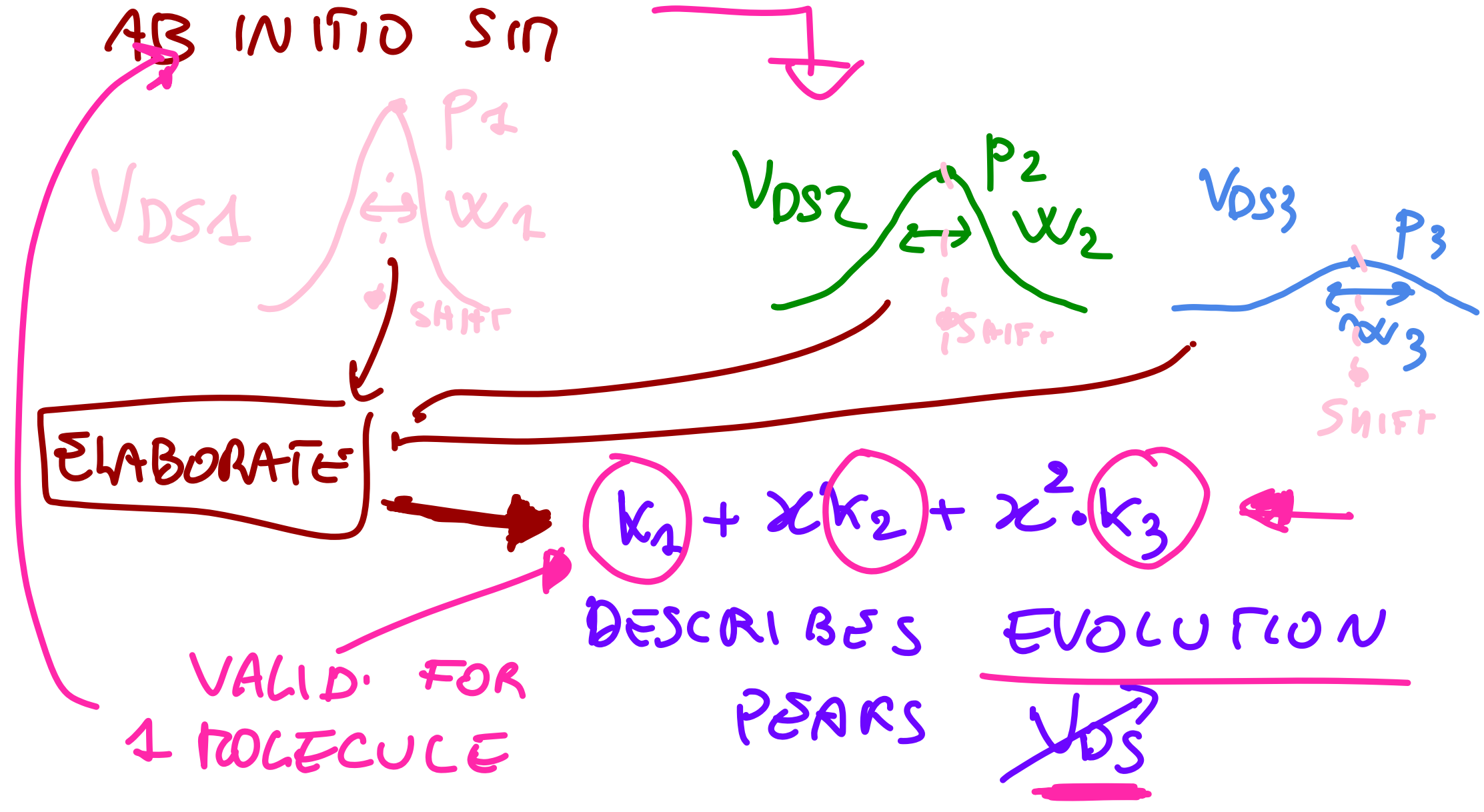


THERE MIGHT BE A PEAK VARIATION .....

TALLER - SLIMMER

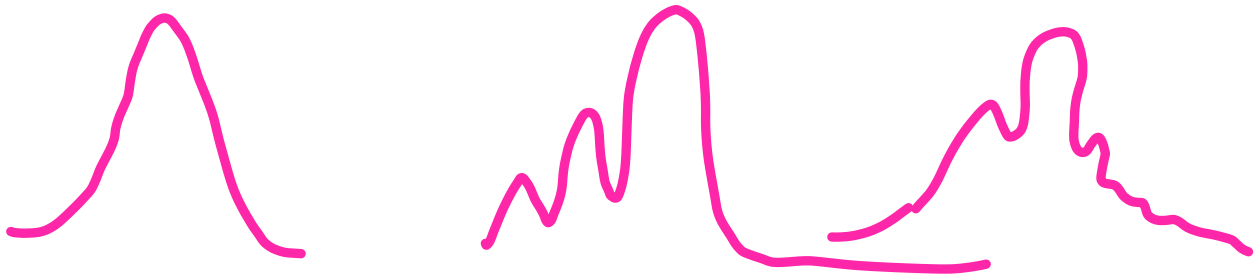
SHORTER - FATTER

TO MODEL ① & ②


AB INITIO SIM
V_{DS1}
P_1
W_1
SHIFT
V_{DS2}
P_2
W_2
SHIFT
V_{DS3}
P_3
W_3
SHIFT
ELABORATE
$k_1 + x k_2 + x^2 \cdot k_3$
DESCRIBES PEAKS
EVOLUTION
V_{DS}
VALID. FOR 1 MOLECULE

OTHER THINGS NOT CONSIDERED FOR NOW

3. PEAKS CHANGE SHAPE



DIFFICULT

4. RESONANCE

EEBESD ORGANIZATION

- INITIAL EVAL @ EQ
- EXTRACTED PARAMS FROM AB INITIO (ESTIMATE DOS K_1 K_2 K_3)

$\forall V_G$ ← α COUPLING FACTOR

$\forall V_{DS}$

↳ EVALUATE E IN SCFL, γ_1 γ_2 ESTIMATE DOS

V_{SCF}

$T(E, V_{DS}, V_{GS})$ $I(V_{GS}, V_{DS})$

FEBSO

USED IN EXERCISES

- FOR SOME MOLECULES
- FOR SEVERAL V_{DS}, V_{GS}
- FOR CASES OF PARAMETERS α, $\lambda_1 \beta_2$

MATLAB BASED

CRISTALLIZATION

a) SCF LOOP

b) SIMPLE CIRCUITS BASED ON IT

→ NEXT LECTURE