EPFL

# MICRO-435 Quantum and Nanocomputing

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FIELD COUPLING NANOCOMPUTING

# FCN

# FIELD COUPLING NANOCOMPUTING

FCN GENERAL VIEW

MOLECULAR IMPLEMENTATION

STRUCTURE & BEHAVIOR

MODEL & CIRCUITS

FABRICATION

# OBJECTIVES

9) FCN GENERAL VIEW

# FCN

## CONCEPT

USE DEVICE NOT AS A

CURRENT-CHANNEL OR SWITCH

BUT AS

STRUCTURED CHARGE CONTAINER

DEVICES ARE ORGANIZED

SO THAT THEY CAN INFLUENCE

EACH OTHER

COUPLING

youtube video

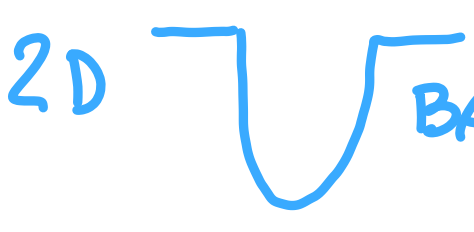
https://youtu.be/Xggg9PzyPdUQ

# PRINCIPLES

1) ENCODE INFORMATION DEPENDING ON WHERE THE CHARGE IS LOCALIZED

2) HAVE A "VESSEL" TO HOST THE CHARGE

ONE POSSIBILITY: QUANTUM DOT




→ 3D QUANTUM CONFINEMENT

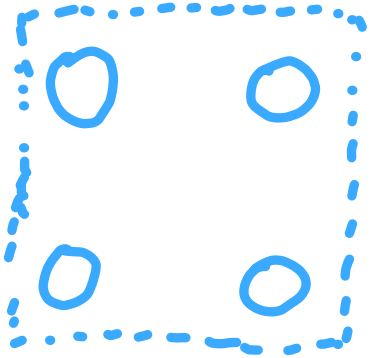
Q.D → SET, LASERS, PHOTODETECTORS

QUANTUM COMPUTING

→ FCN { Q.DOT, MOLECULAR QD, MAGNETIC } Q.D

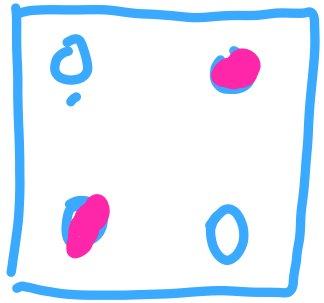
# BASIC CONCEPTS, FOR NOW GENERIC QUANTUM DOTS

BASIC ELEMENT



4 Q.D. FORM A SQUARE

'1' '1'



2 POSSIBLE STABLE STATES

2 ELECTRONS

↓

THEY WILL OCCUPY 1 DOT EACH

↓

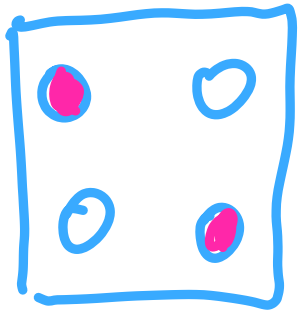
OCCUPY THE DIAGONAL DUE TO COULOMB REP.

↓

LOWER ENERGY

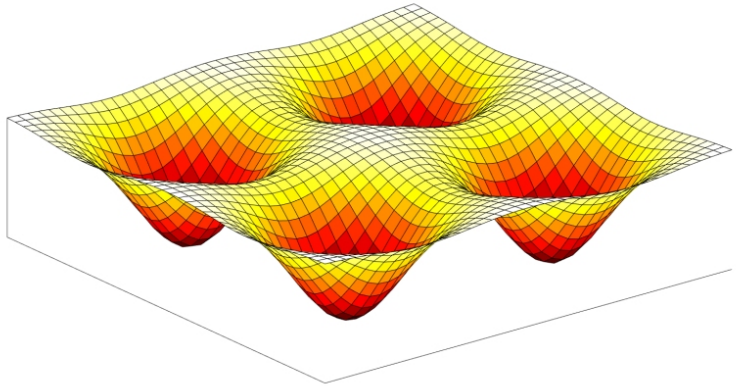
ENCODED '0' '1' BINARY INFO!

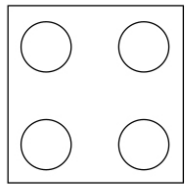
'0' '0'

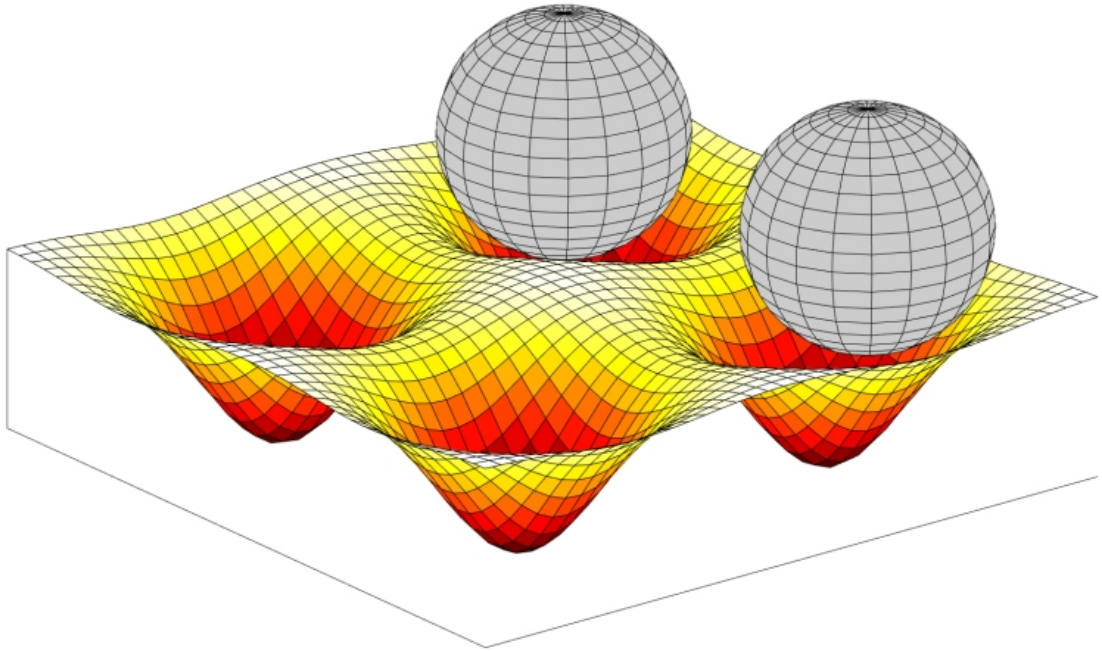


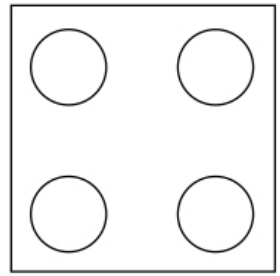
ENERGETICALLY EQUIVALENT

CONCEPTUAL VIEW



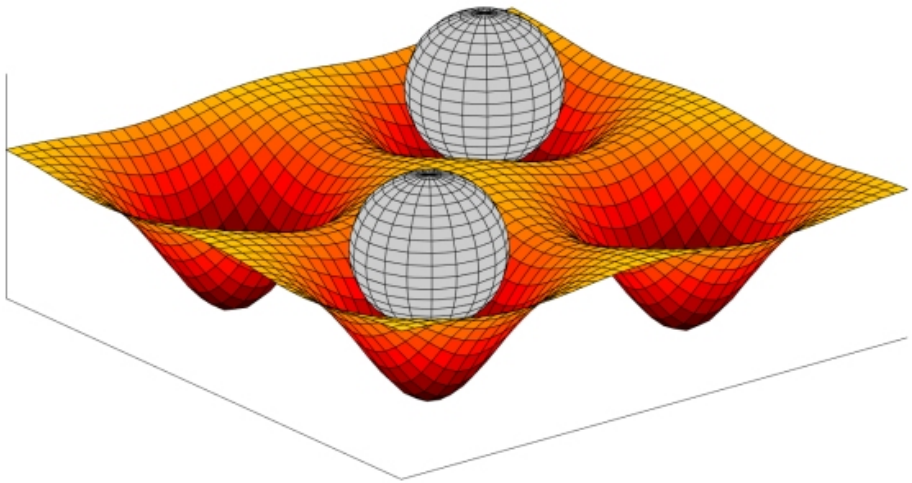


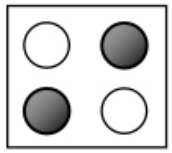




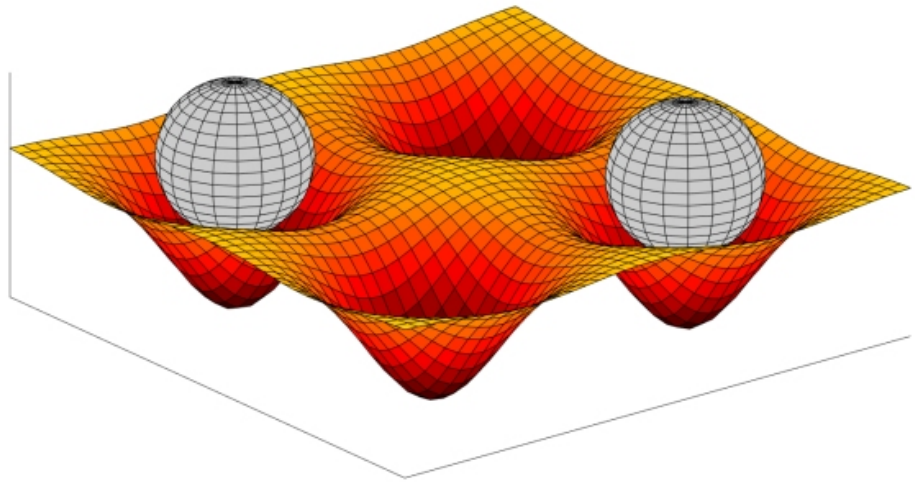
2 Coulomb charges

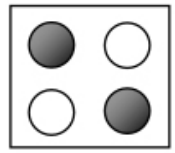
# CONCEPTUAL VIEW





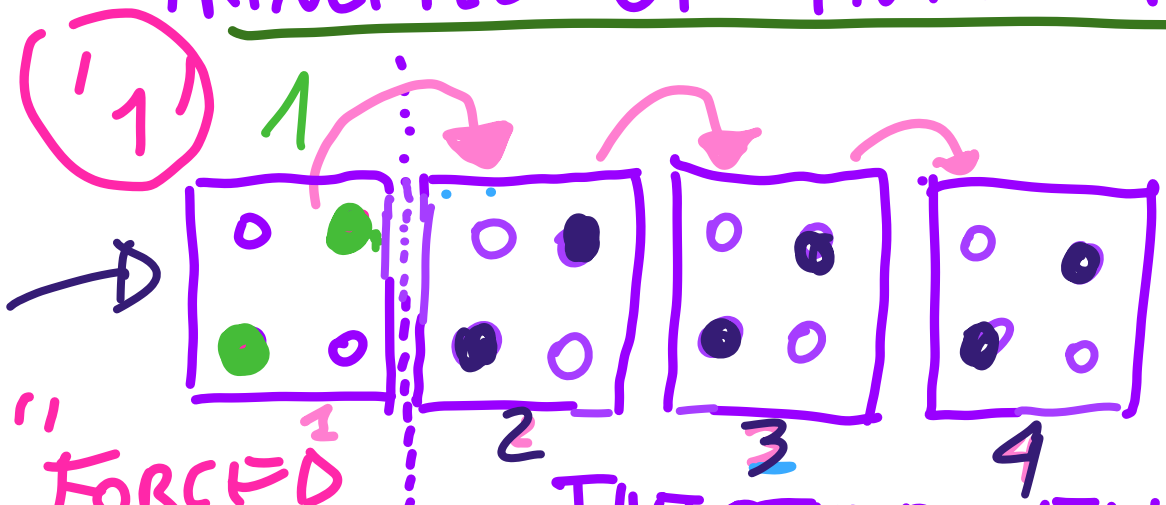
'1'





'0'

# PRINCIPLE OF INFO PROPAGATION



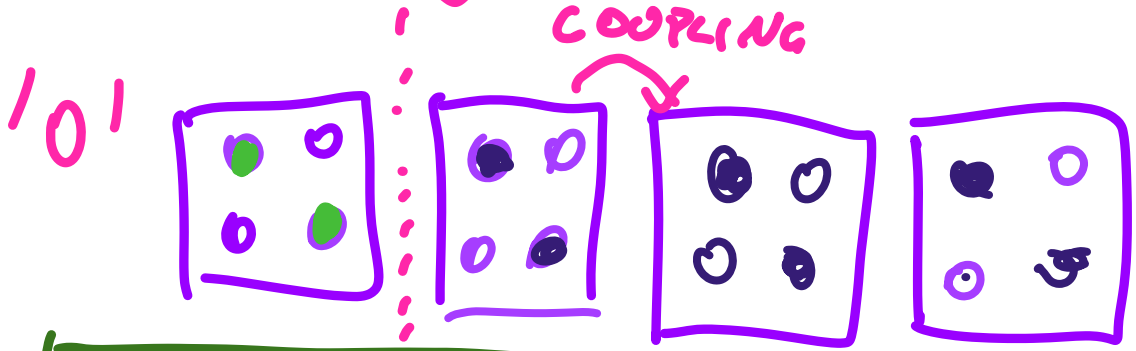

PLACE CELLS AT THE CORRECT DISTANCE

"FORCED STATE" INPUT

THE OTHER CELLS HAVE "FREE CHOICE"

THE CONF. WILL ASSUME THE SAME OF THE INFO → DOMINO STYLE

FOLLOW LOWEST ENERGY STATE




WIRE OF CELLS

- CHARGES MOVE ONLY WITHIN THE CELL
- INFO PROP. THROUGH COUPLING

NO CHARGE TRANFER BW CELLS!

LOW POWER DISSIPATION

↳ ENERGY TO TRANFER CHARGES FROM '1' ⇄ '0'

$\sim 1 \cdot 10^{-20}$ J

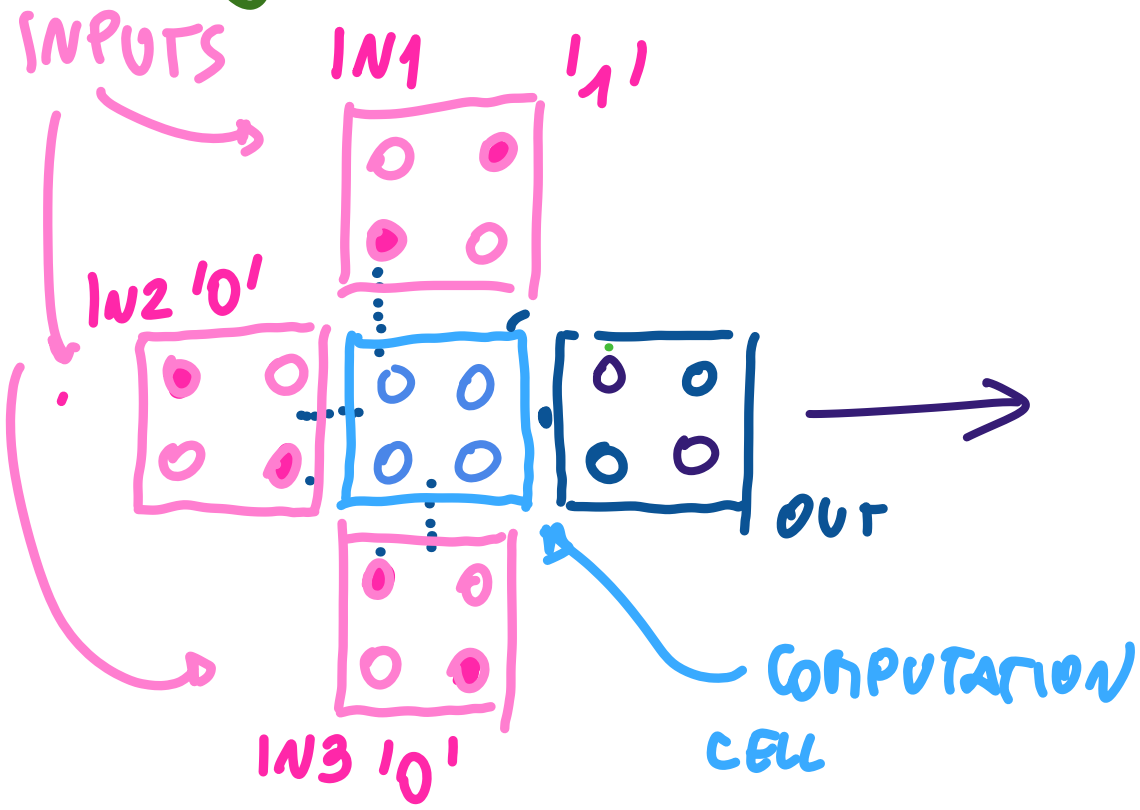
FOR A MINIMUM SIZE TRANSISTOR SWITCH $1 \cdot 10^{-18}$ J

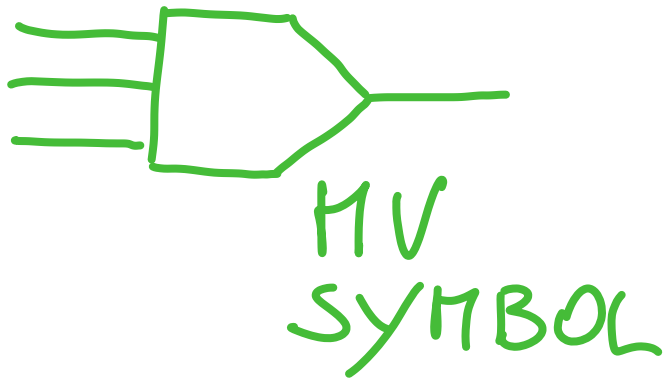
# LOGIC FUNCTIONS?

↓

OBTAINED BY SPECIFIC PLACEMENT OF CELLS

## MAJORITY VOTER



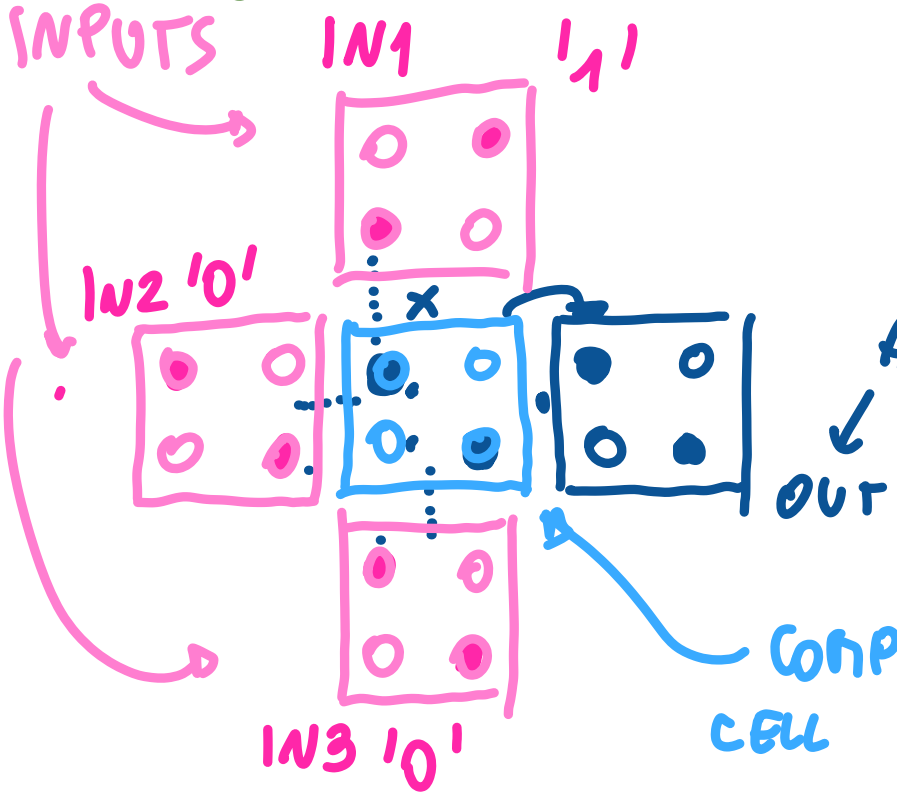

TRY!

# LOGIC FUNCTIONS.

↓

OBTAINED BY SPECIFIC PLACEMENT OF CELLS

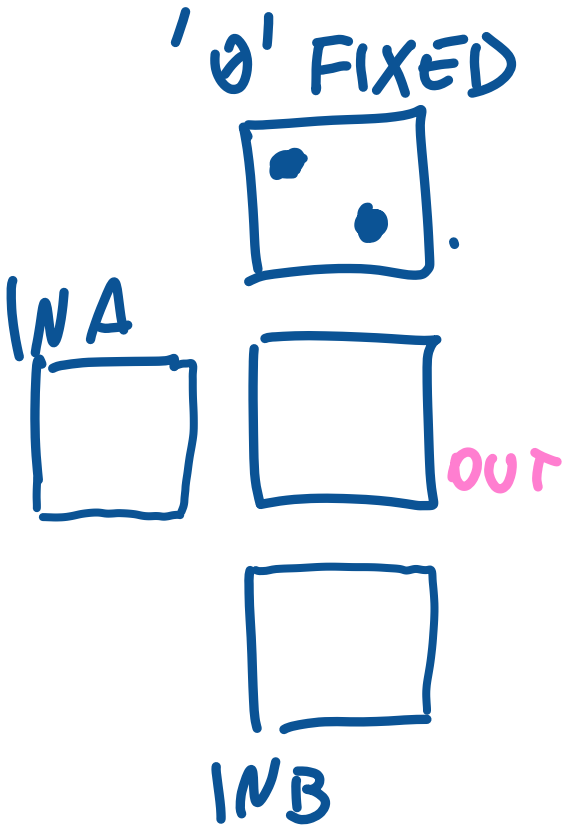
## MAJORITY VOTER



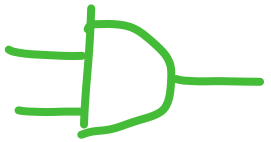

ASSUMES THE VALUE OF COMP. CELL

TRY!

# HOW TO OBTAIN AND, OR?

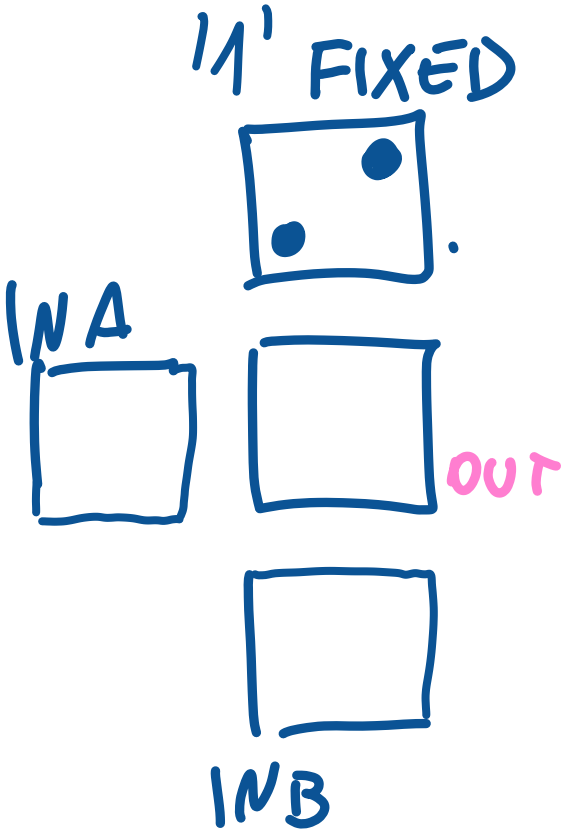



| INA | INB | OUT |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 0 |
| 1 | 0 | 0 |
| 1 | 1 | 1 |

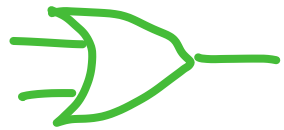
AND 

CAN BE EXPLOITED FOR "COFIGURABILITY"

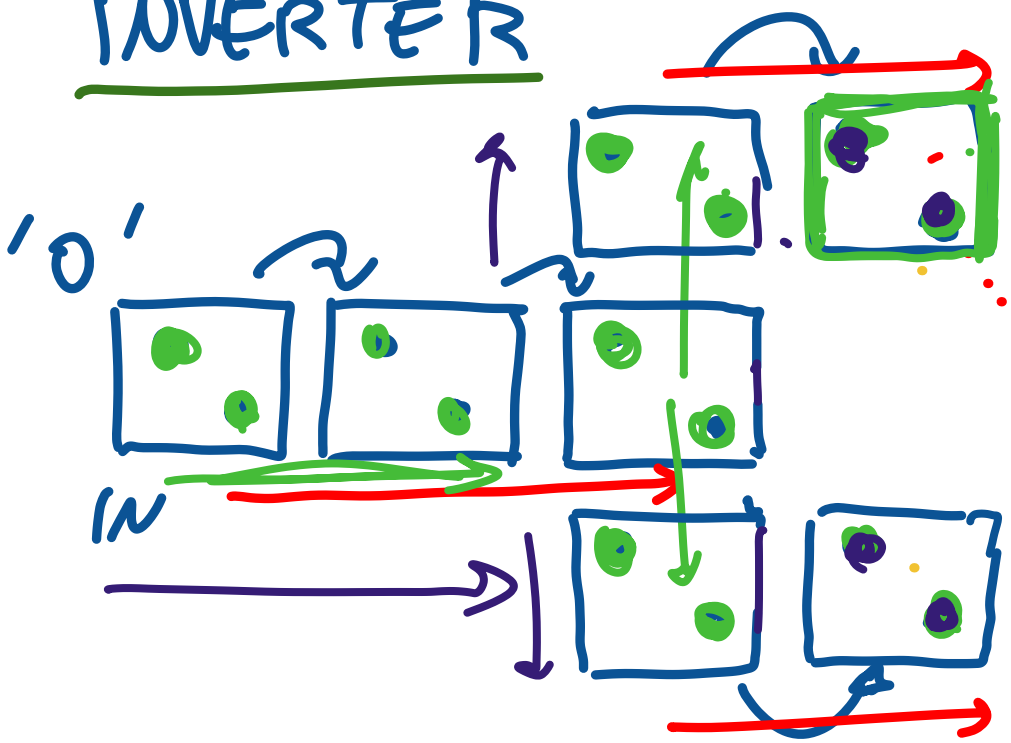
# HOW TO OBTAIN AND, OR.

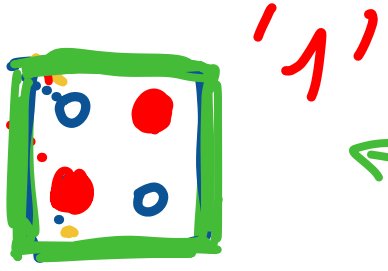


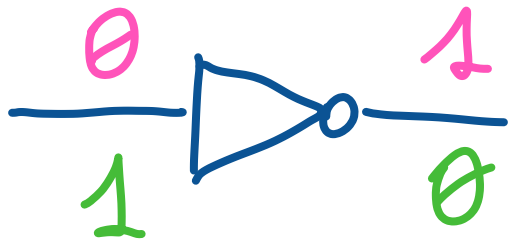

| INA | INB | OUT |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 1 |

OR 

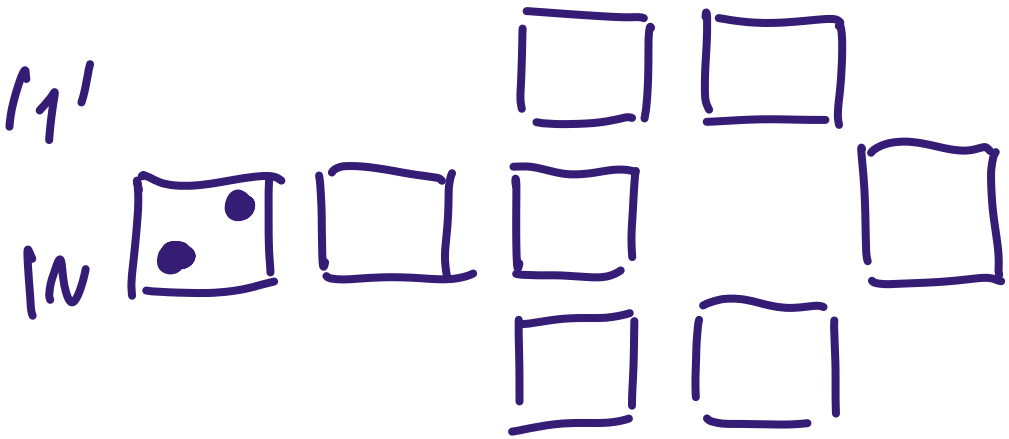
# INVERTER

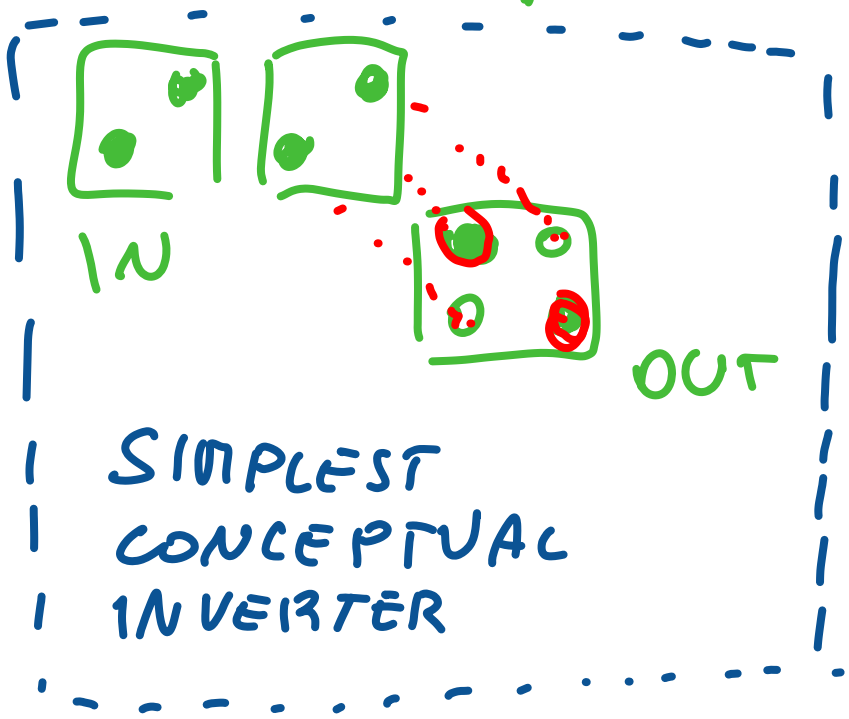


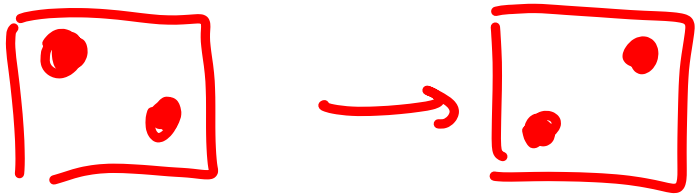

TRY OPPOSIT CASE



# IMPORTANT CONSIDERATION

→ WE WANT TO SWITCH A CELL



ASSUME LOW POTENTIAL BARRIER BW 2 CONFIG

→ WE WANT STABLE LOGIC VALUES

ASSUME A HIGH POTENTIAL BARRIER BW 2 CONF

→ ASSUME DIRECTION OF INFO PROP.
EX. FROM LEFT TO RIGHT

→ ASSUME NO LOSS OF INPUT PROP

# TO ASSURE CORRECT INFO PROP.

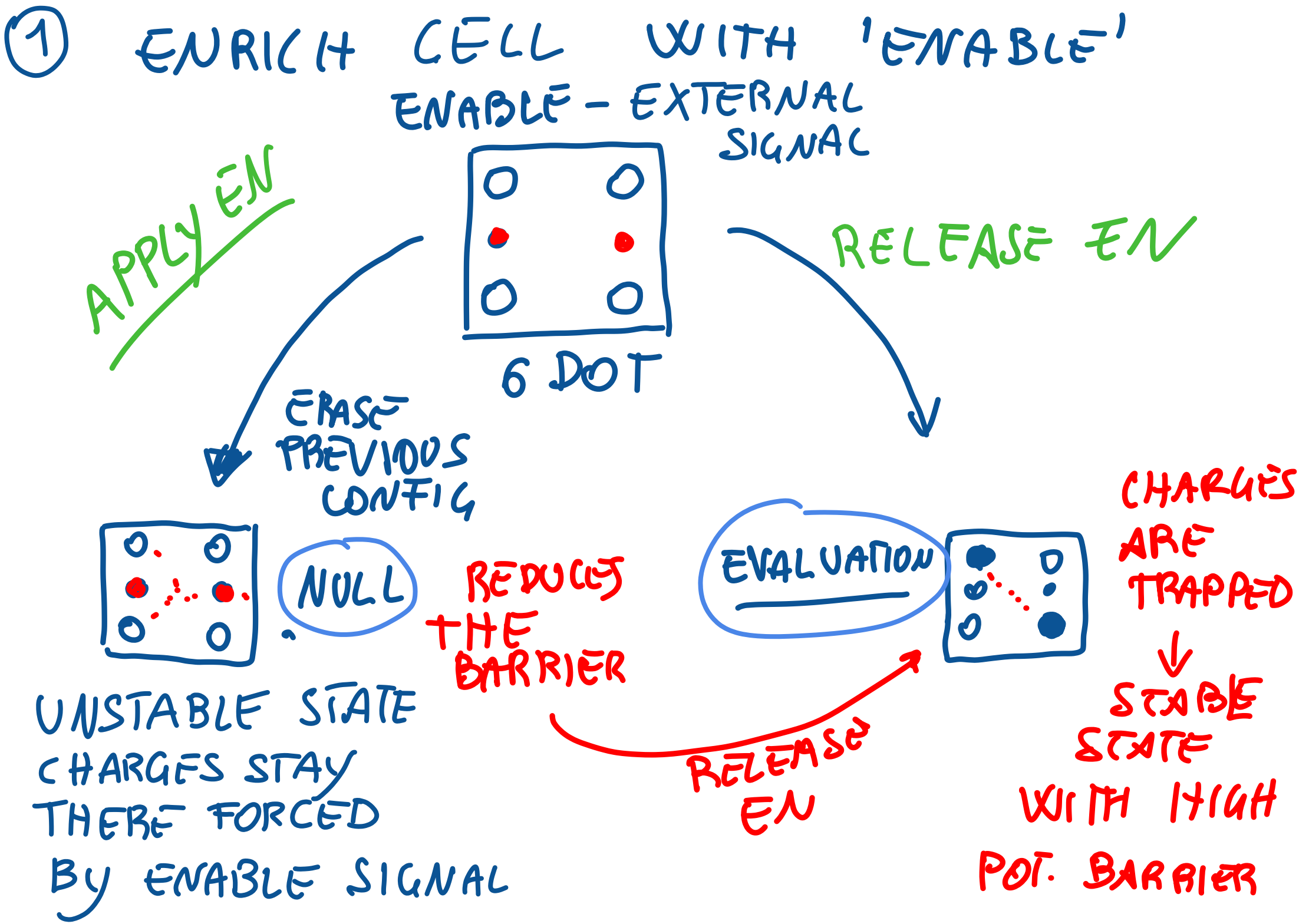
1. – ENRICH THE CELL WITH A FURTHER DOT
   ↳ USE EXTERNAL "ENABLE" SIGNAL
   TO FAVOR THE SWITCH

2. – CIRCUITS ORGANIZED IN ZONES

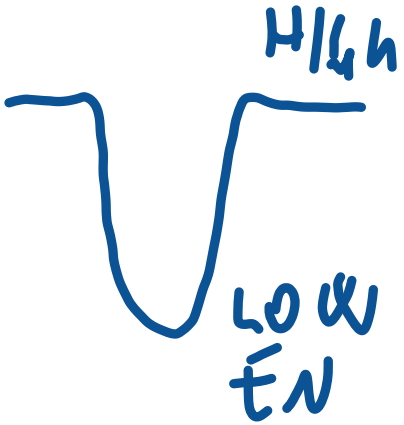
3. – EACH ZONE WITH A CERTAIN N° OF CELLS

4. – EACH ZONE HAS A SPECIFIC ENABLE, APPLIED WITH CERTAIN SEQUENCE

⇒ INFO PROPAGATES IN PIPELINE


1 ENRICH CELL WITH 'ENABLE'
ENABLE - EXTERNAL SIGNAL
APPLY EN
6 DOT
RELEASE EN
ERASE PREVIOUS CONFIG
NULL
REDUCES THE BARRIER
EVALUATION
CHARGES ARE TRAPPED
STABLE STATE WITH HIGH POT. BARRIER
RELEASE EN
UNSTABLE STATE CHARGES STAY THERE FORCED BY ENABLE SIGNAL

# ① ENERGY CONSIDERATIONS




DIRECT TRANSITION MEANS TO SPEND A CERTAIN ENERGY

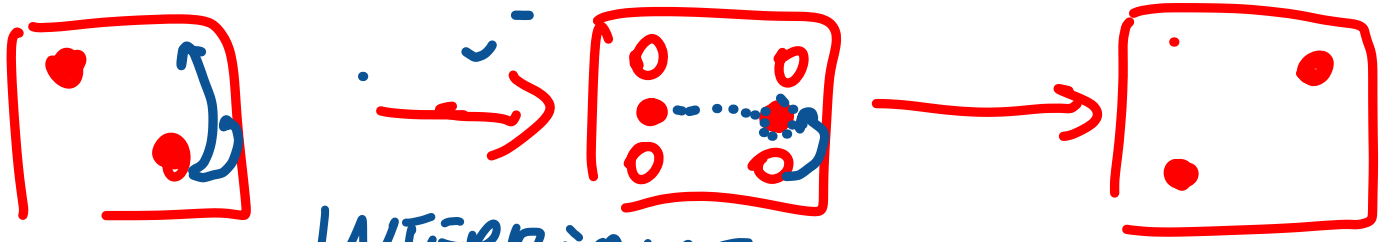
STABLE

STABLE

# ① ENERGY CONSIDERATIONS

THE TOTAL ENERGY IS SMALLER THAN THE DIRECT CASE.

WE APPLY EXT. EN IN ADIABATIC WAY



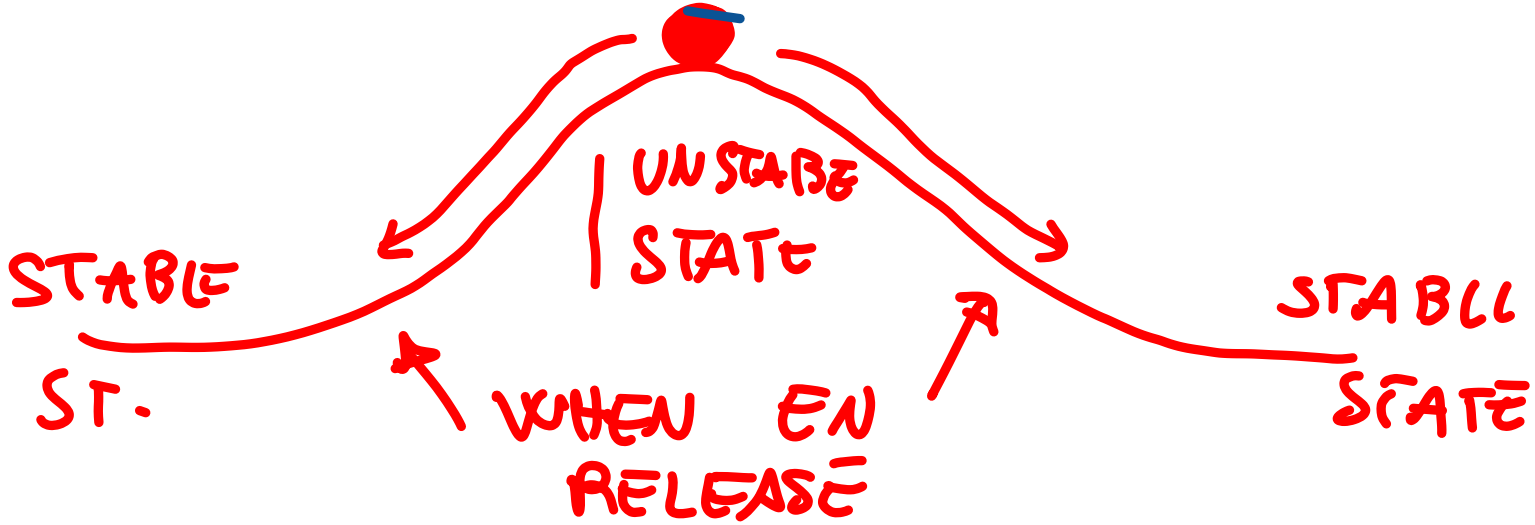
INTERMEDIATE EN. LEVEL

INT. EN.

SPEND ENERGY TO GO THE NULL

↓

NEW EVAL



# ① ENERGY CONSIDERATIONS

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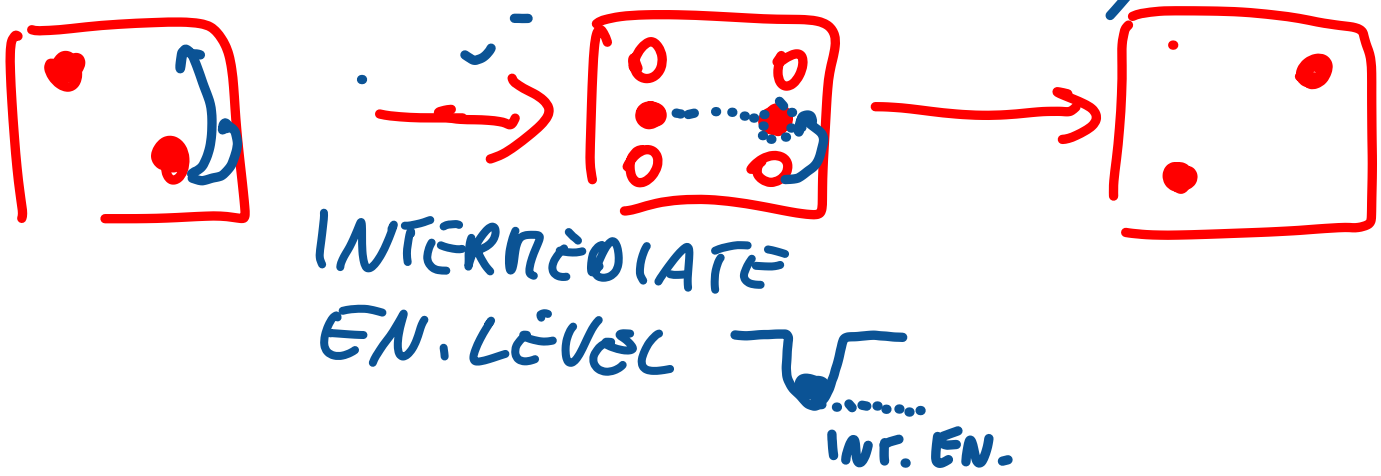
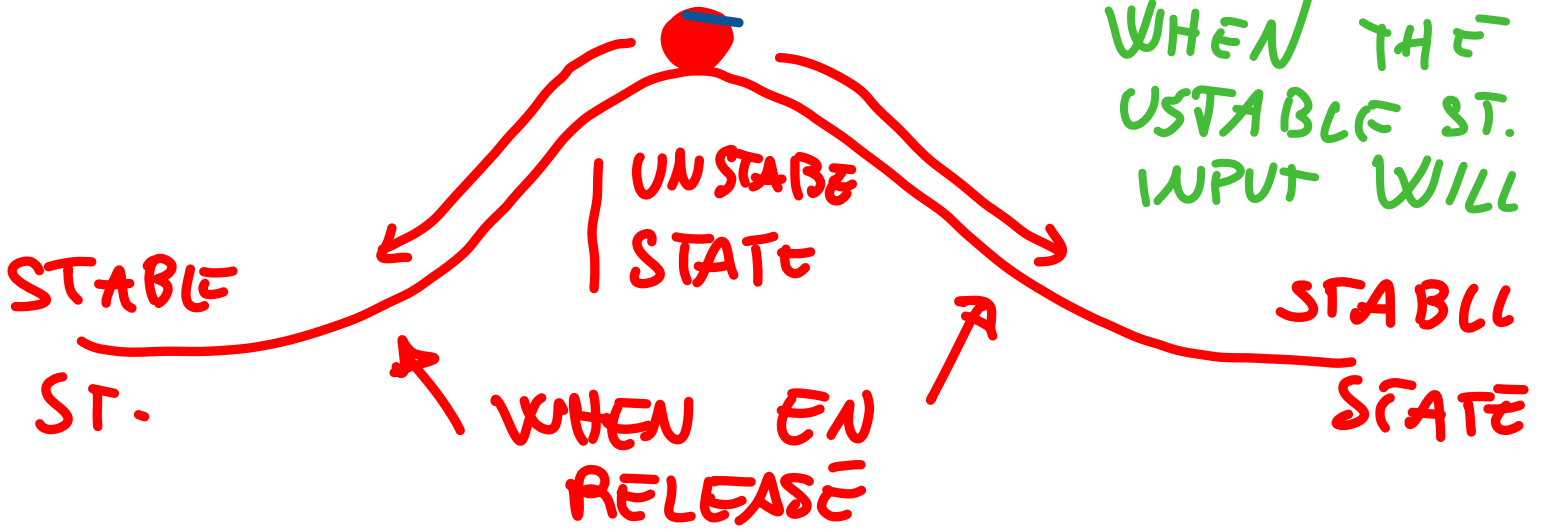



SPEND ENERGY TO GO THE NULL ↓ NEW EVAL




WHEN THE USTABLE ST. EVERY INPUT WILL FAVOUR "1" OR "0"

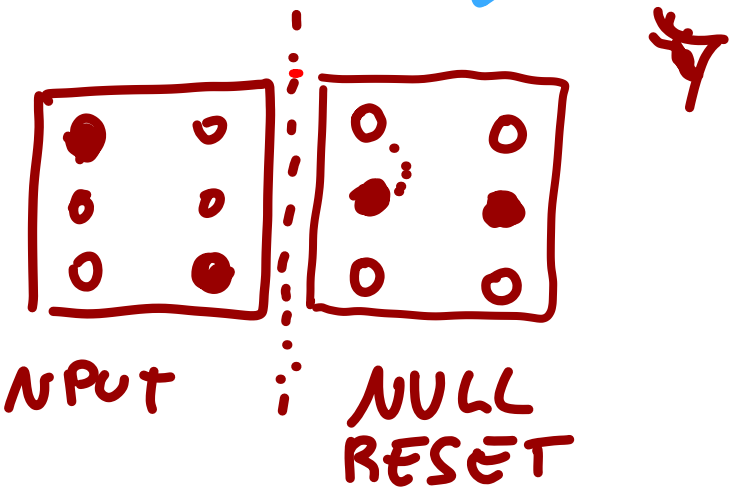
(2)

EXTERNAL FIELD

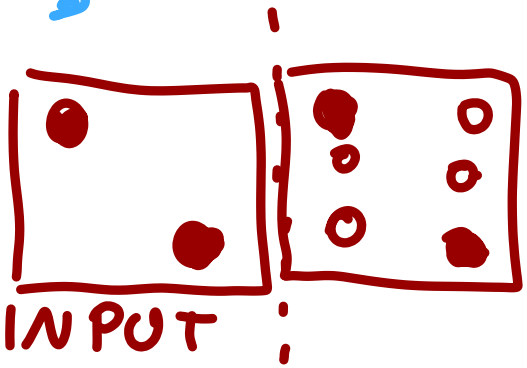
APPLIED | RELEASED | APP. | REL

A R

SIMILAR TO "CLOCK"



INPUT | NULL RESET

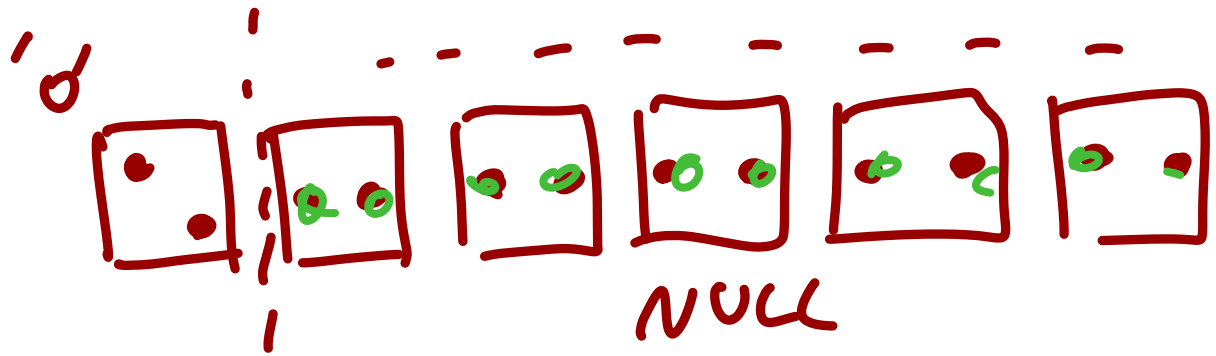


CHARGES WILL GO IN ONE OF THE 2 STABLE STATES

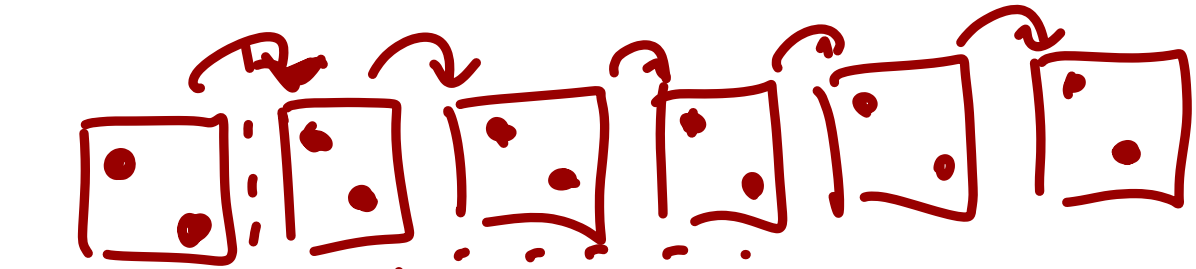
INPUT

THE INPUT INFLUES WHICH STATE

(2)




A TO ALL

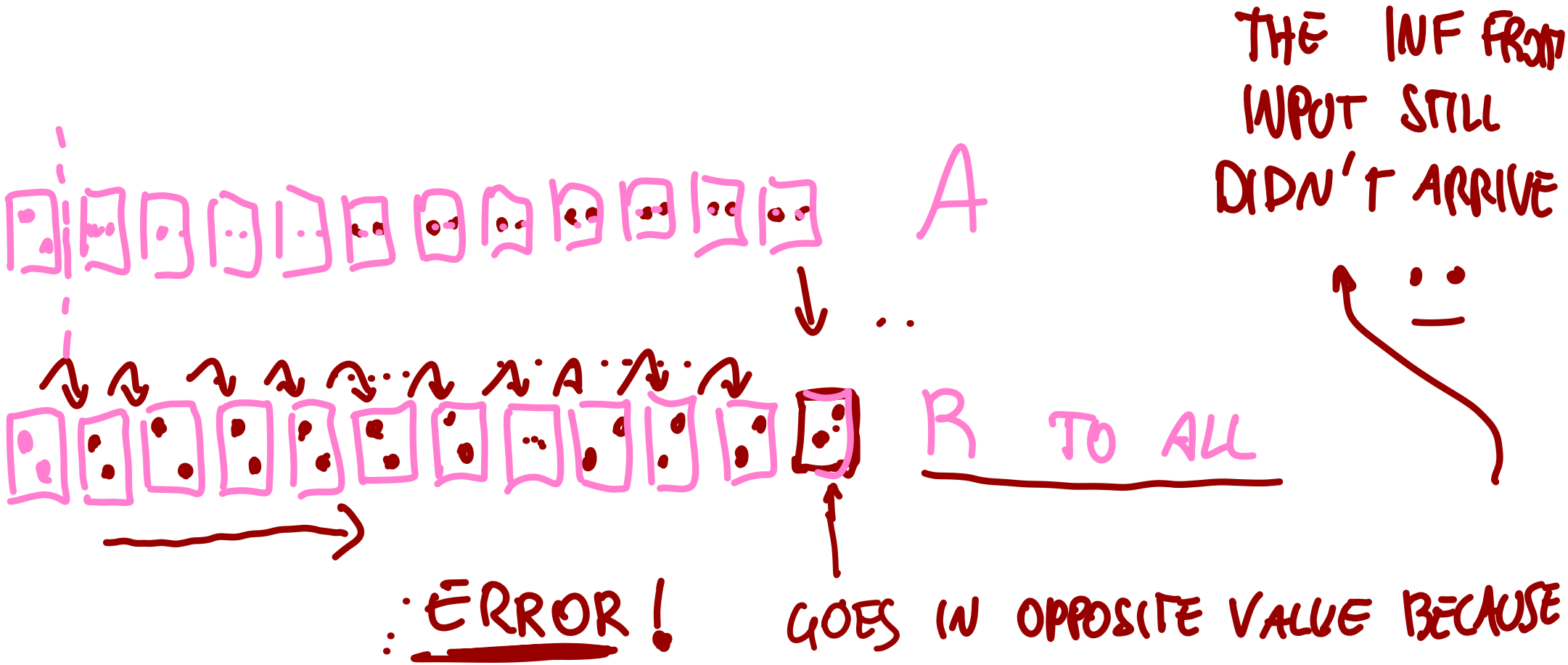


R TO ALL

SIMILAR IN OPPOSITE CASE

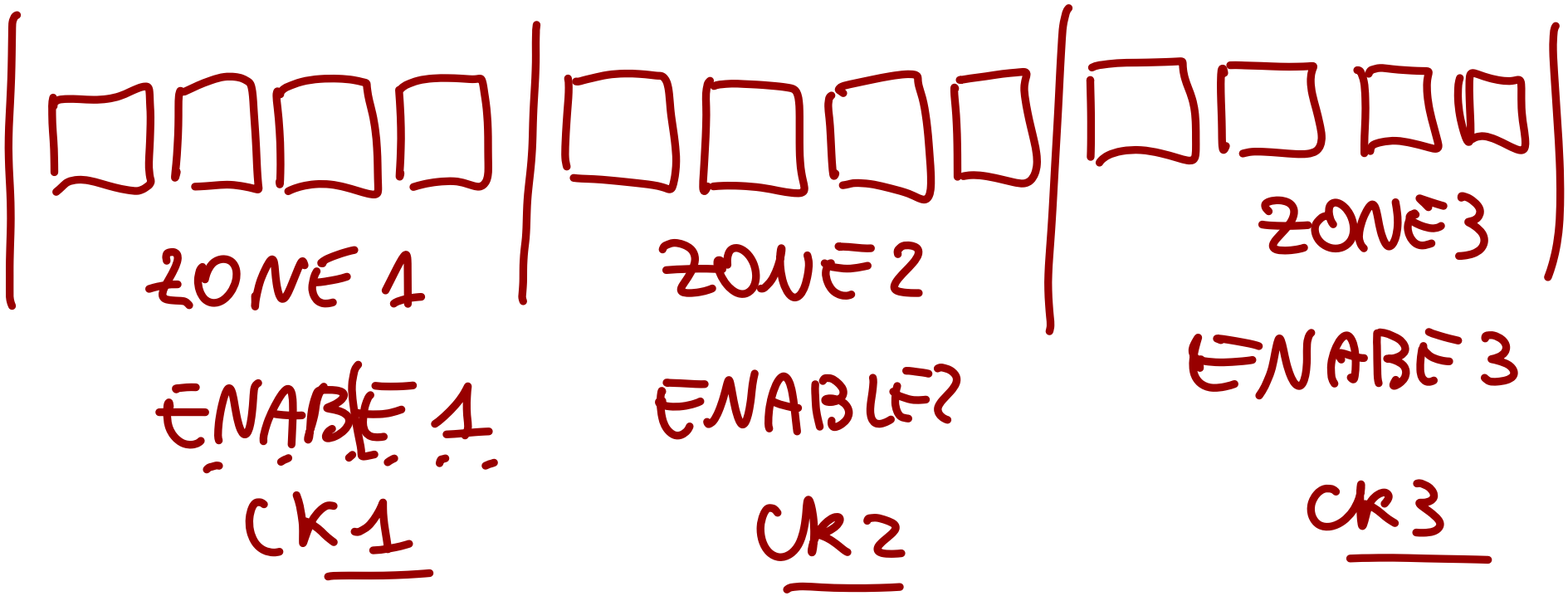
3

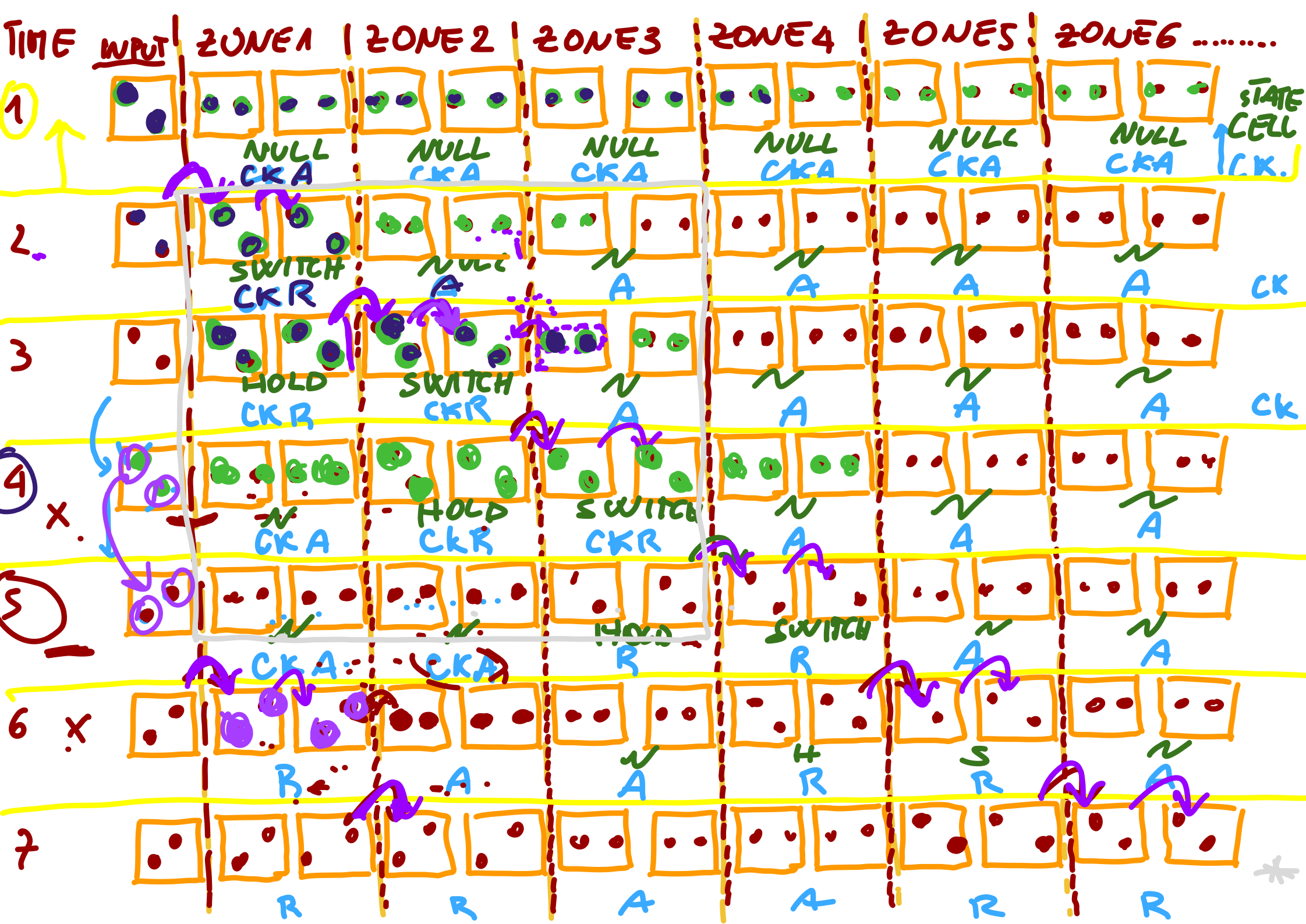
# THE CASE OF A LONG CELL SEQUENCE

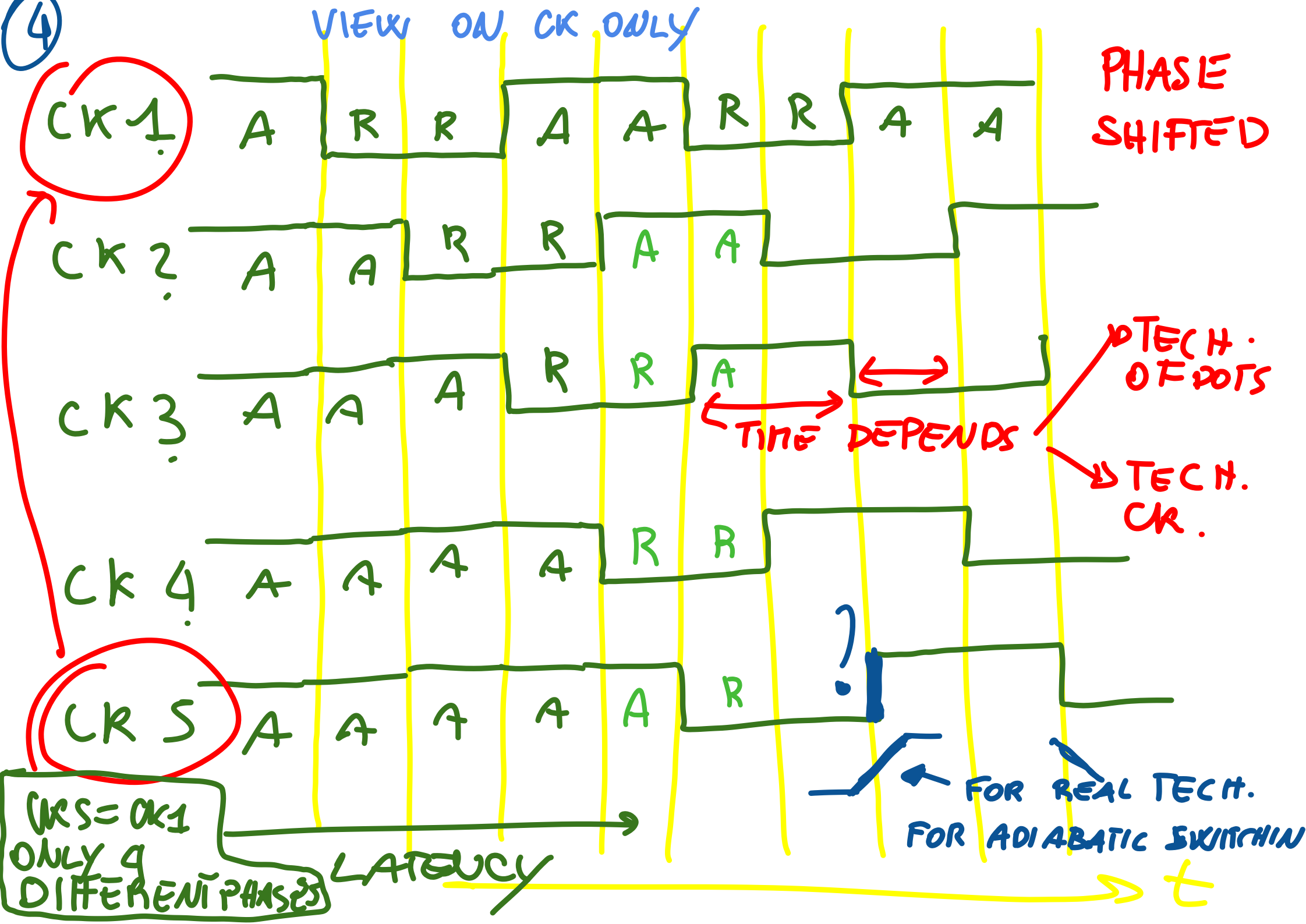


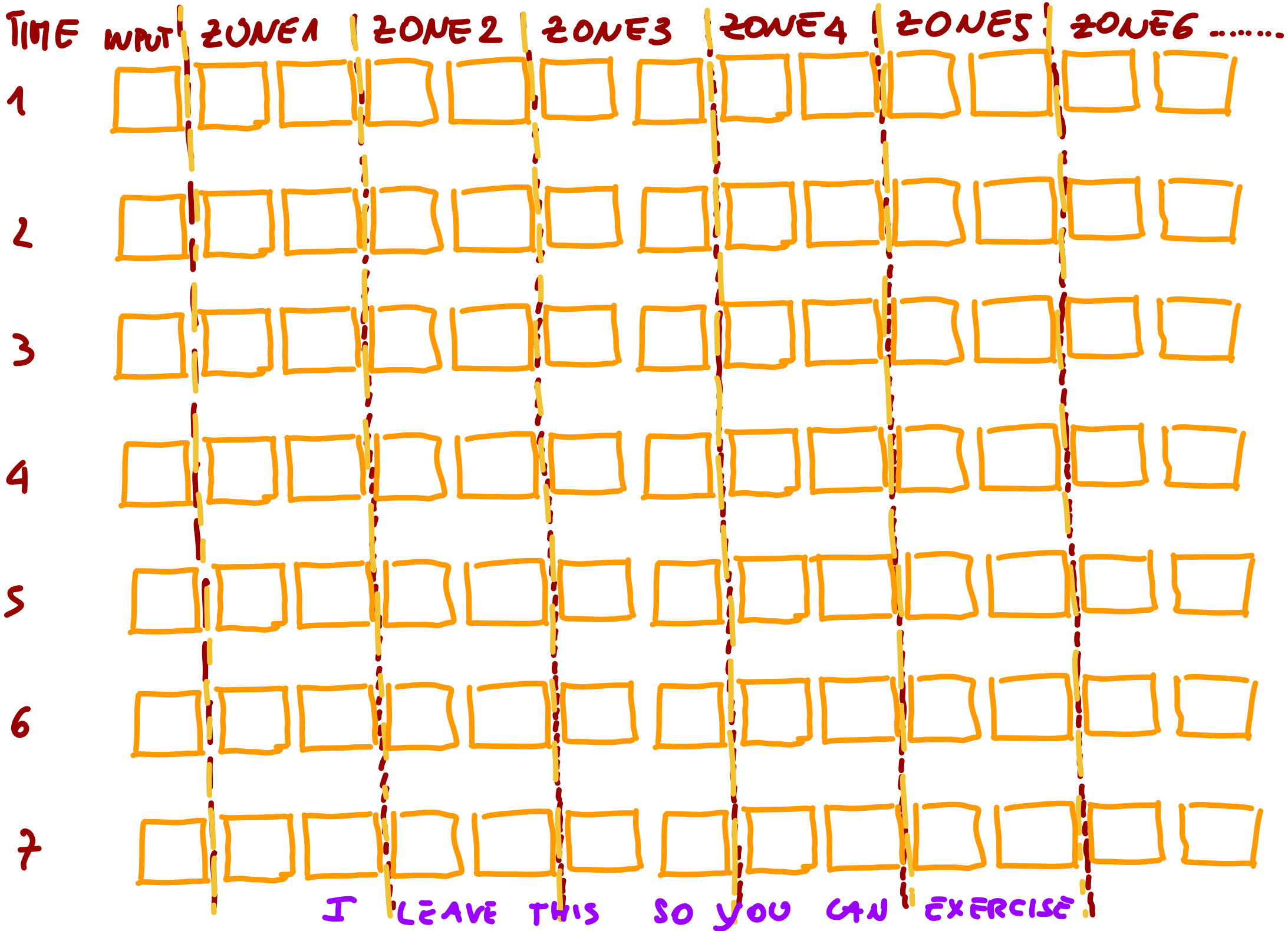
(3)

ZONES WITH THESAME (EN) APPLIED CAN HOST ONLY A LIMITED N° OF CELLS



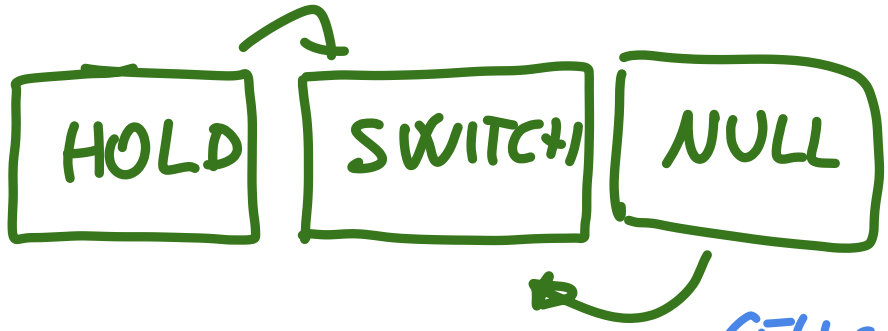

TIME
INPUT
ZONE1
ZONE2
ZONE3
ZONE4
ZONE5
ZONE6 .....
STATE CELL CK.
NULL CKA
SWITCH CKR
HOLD CKR
SWITCH CKR
CK
Ck
CKA
R
A
S


4
VIEW ON CK ONLY
PHASE SHIFTED
CK1
CK2
CK3
CK4
CK5
A R R A A R R A A
A A R R A A
A A A R R A
A A A A R R
A A A A A R
TECH. OF DOTS
TIME DEPENDS
TECH. CK.
?
FOR REAL TECH.
FOR ADIABATIC SWITCHIN
CK5=CK1
ONLY 4
DIFFERENT PHASES
LATENCY
t


TIME
INPUT
ZONE1
ZONE2
ZONE3
ZONE4
ZONE5
ZONE6 .....
1
2
3
4
5
6
7
I LEAVE THIS SO YOU CAN EXERCISE

(4)

→ BEFORE RELEASING THE 4CK IT IS NECESSARY TO BE SURE THAT THE CELLS IN THE FOLLOWING ZONES ARE IN NULL STATE!




INFO PROP DIRECTION →

↑ PREVIOUS CELLS CAN GO IN NULL PHASE

CELLS IN NULL DO NOT INFLUENCE THE SWITCHING CELLS THAT FOLLOW THE CELLS IN HOLD AS INPUT

# OBJECTIVES

b) FCN MOLECULAR IMPLEMENTATION

# POSSIBLE IMPLEMENTATIONS

- METALLIC SET → WORK ONLY AT VERY LOW TEMP
- HETEROSTRUCTURE (USED FOR LASERS)
- MAGNETIC (SEVERAL FLAVOURS) → LATER
- MOLECULAR → WORK AT ROOM TEMP
  - → SMALL
  - → SELF ASSEMBLY
  - → VERY LOW POWER
  - → SWITCH TIME VERY HIGH! → ASSURE HIGH FREQ ≫ 10THz

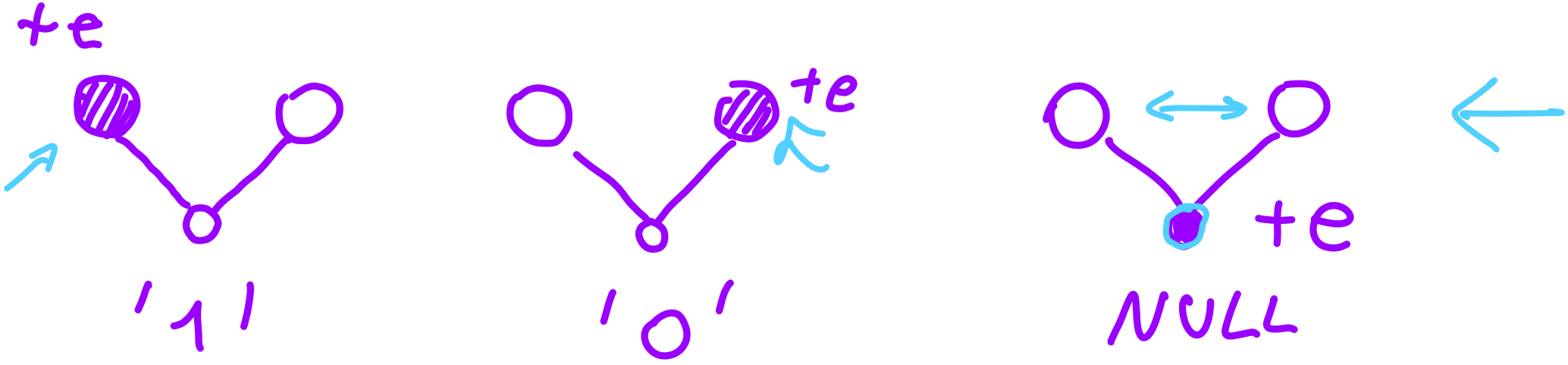
# FCN MOLECULAR IMPLEMENTATION

## CONCEPTUAL MOLECULE FOR FCN

- 3 **DOTS** AT LEAST — HALF CELL
- DOT → REDOX CENTER

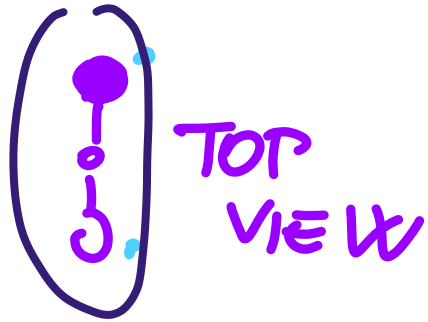
REDUCTION — OXIDATION

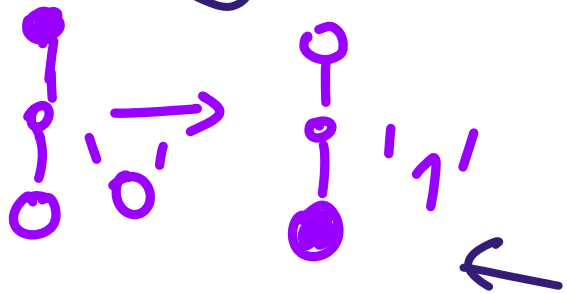
GAIN 1 el. — LOSS 1 EL

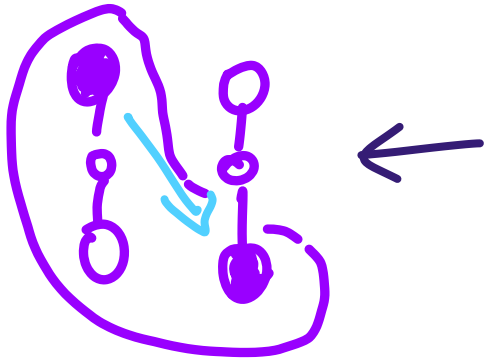


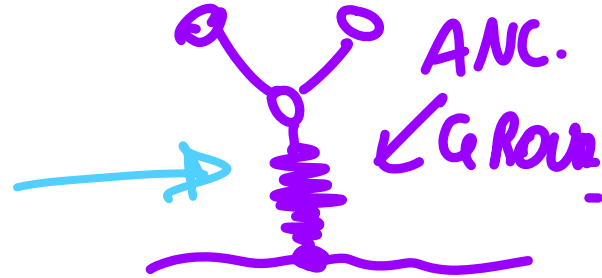
# KEY REQUIREMENT

- CHARGE LOCALIZATION
- CHARGE SWITCHING
- COUPLING THROUGH COULOMB REP. → FOR PROPAGATION
- SENSITIVITY TO UK
- ALLOW ANCHORING

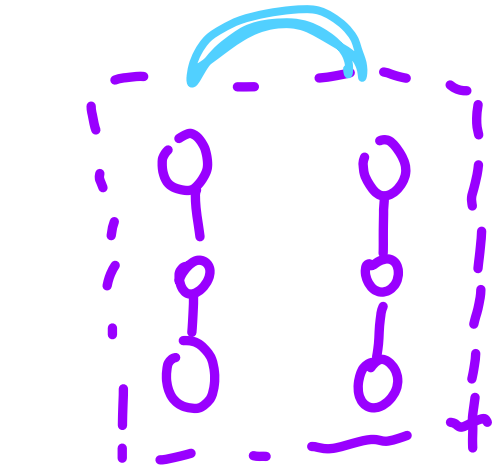


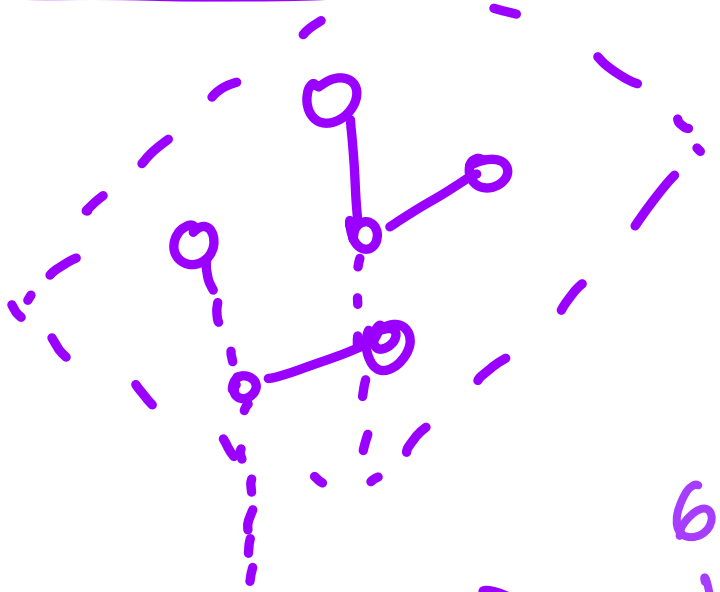





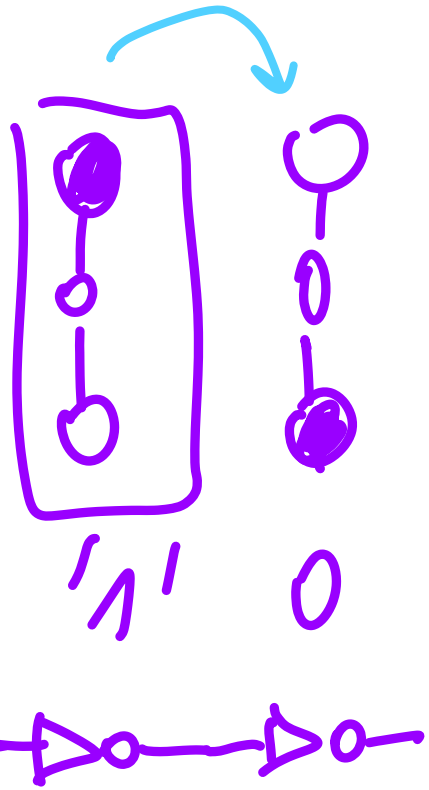
# UNITS OF INFORMATION

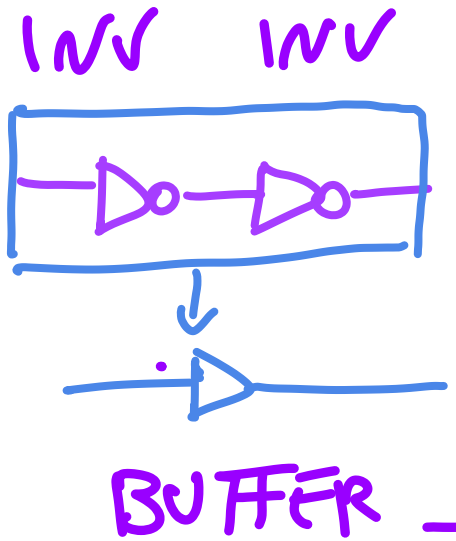


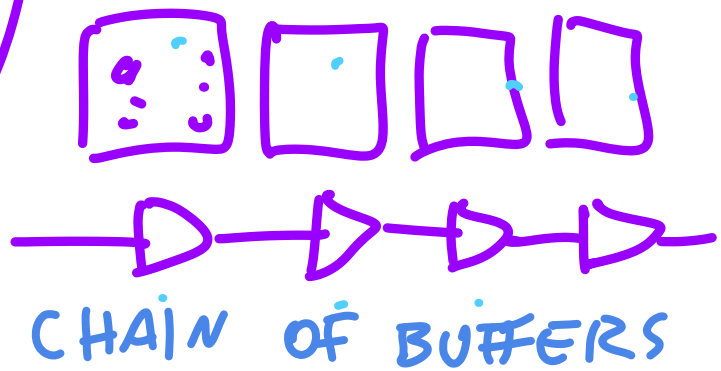


3 DOTS MOLECULE EASY TO SINTH

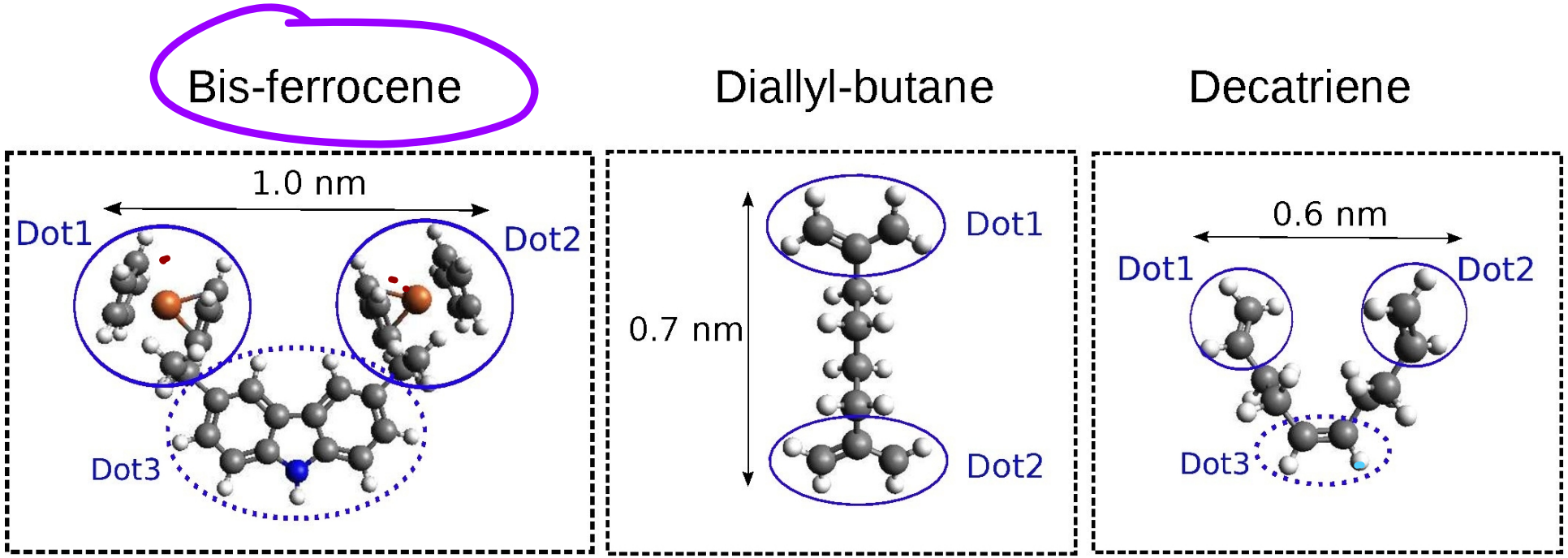
6 DOTS MOL. VERY DIFFICULT TO SYNTH.



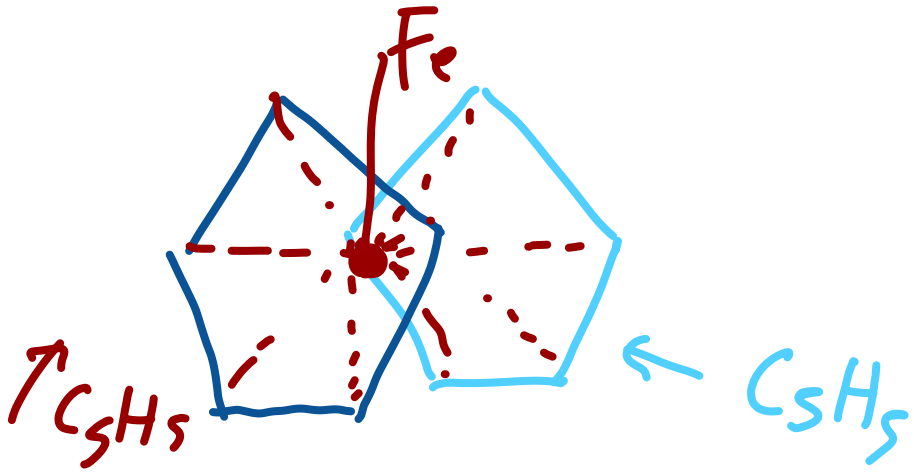



# SOME OF THE POSSIBLE MOLECULES FOR FCN



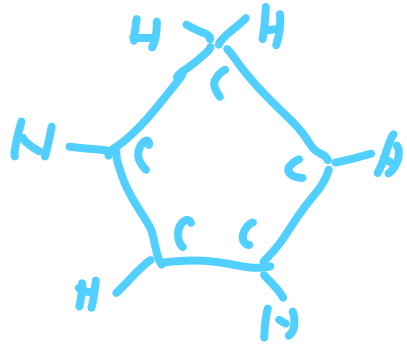
# FERROCENE

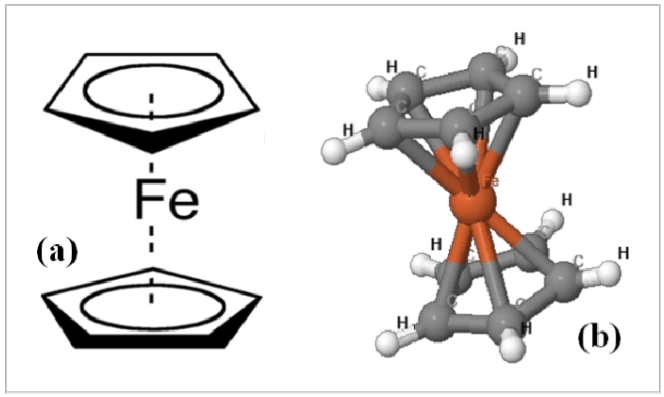
$Fe(C_5H_5)_2$

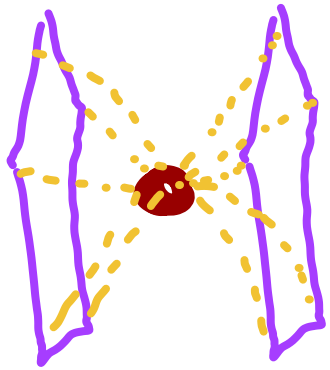


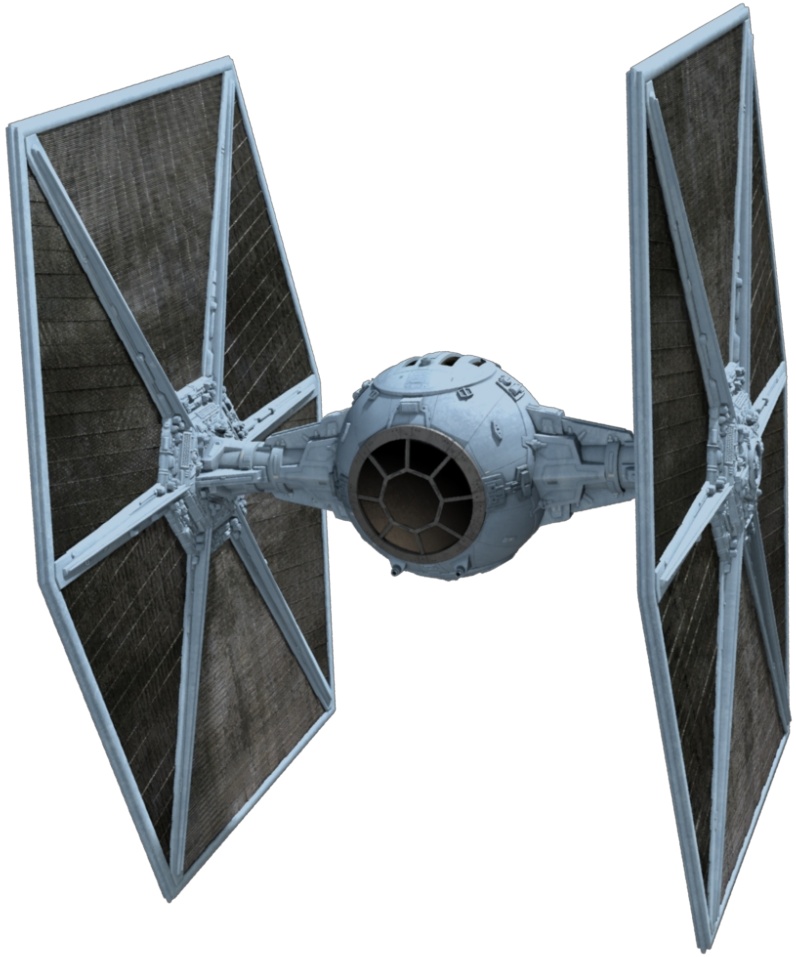

CYCLOPENTADIENE

$C_5H_6$



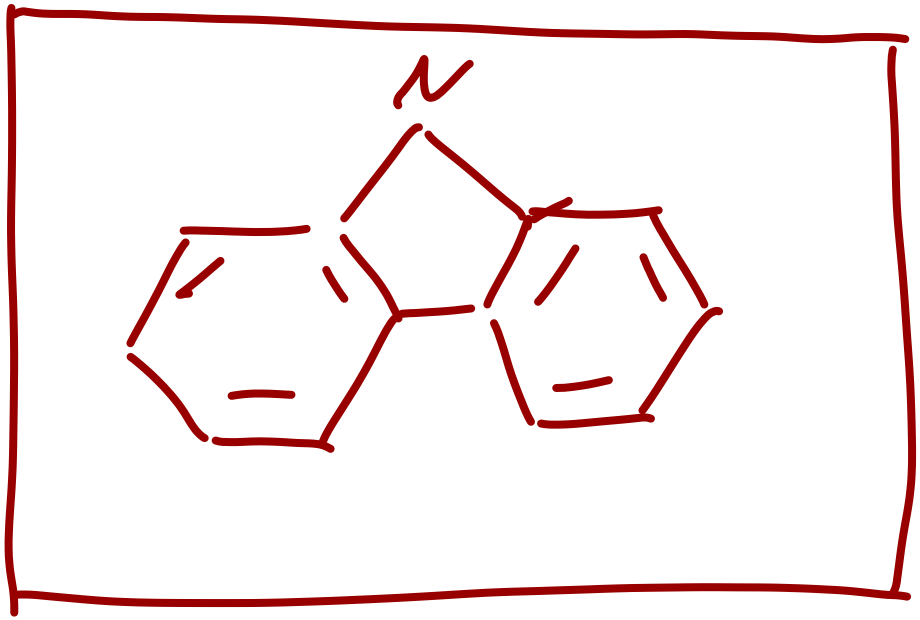




Do you recognize it?

# CARBAZOLE $C_{12}H_9N$

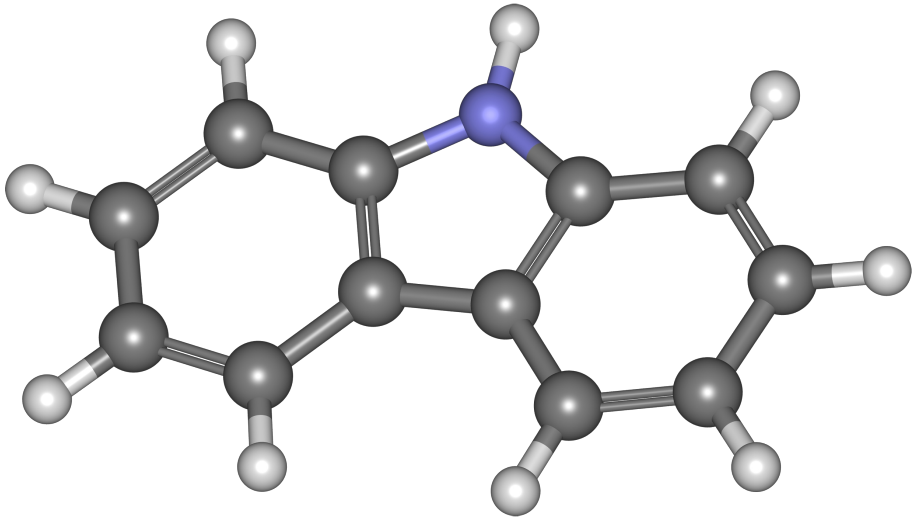



IF TAKEN
STAND ALONE

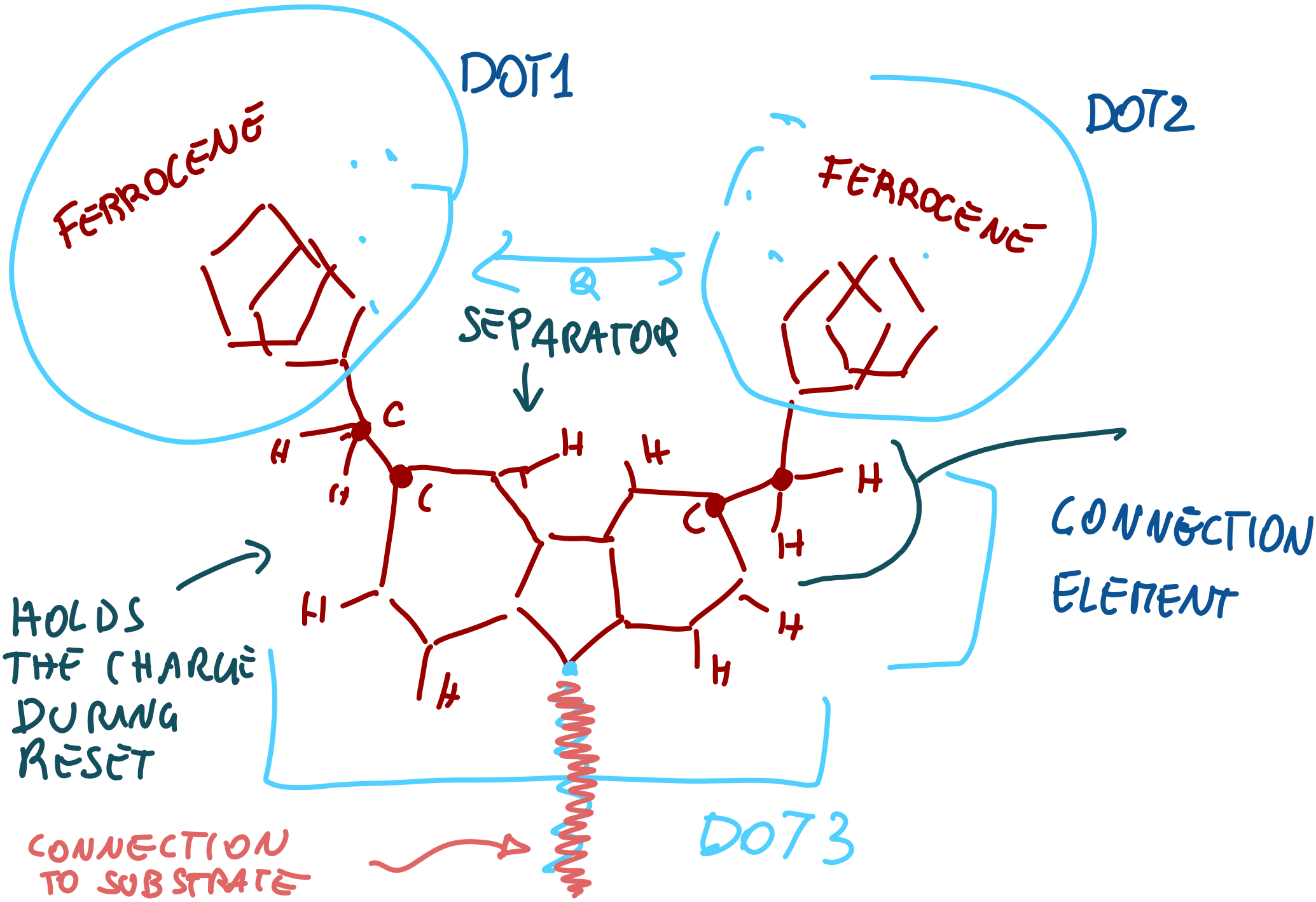
IT CONNECTS TO
FERROCENE LOOSING H

AND THROUGH A

$CH_3$ ELEMENT

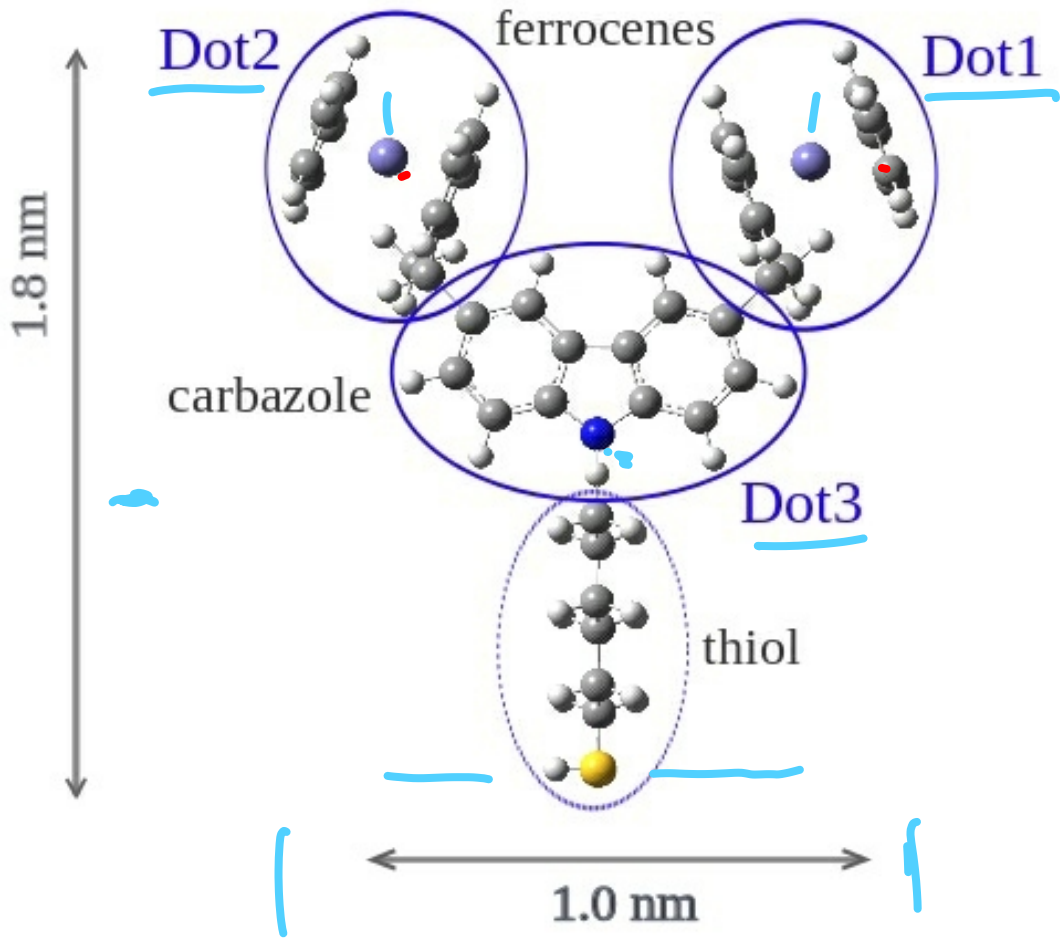


# PUTTING IT ALL TOGETHER



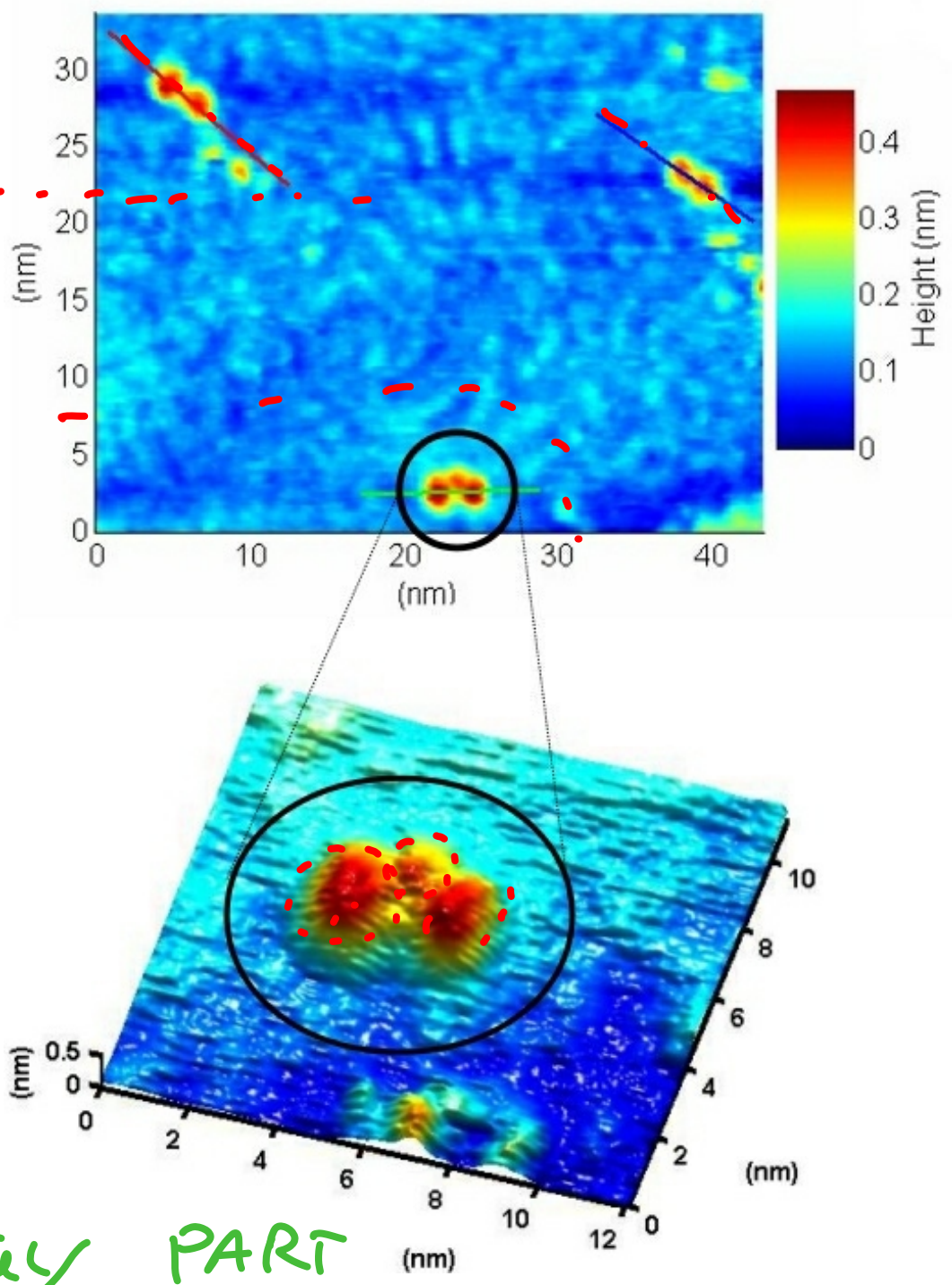
SWITCH E.F.

BISFERROCENE AS FCN UNIT CELL HOWTO



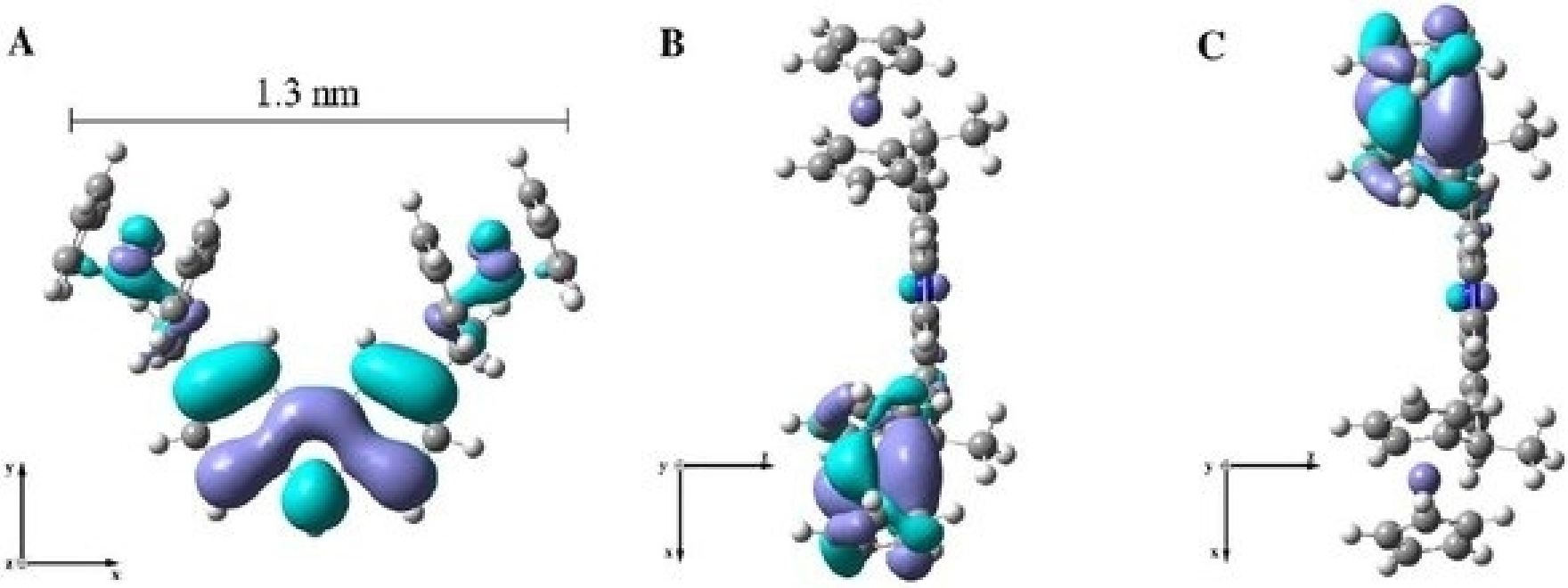

CLOCK E.F

STM VIEW OF MOLECULE DEPOSITED ON GOLD




SEE LATER TECHNOLOGY PART

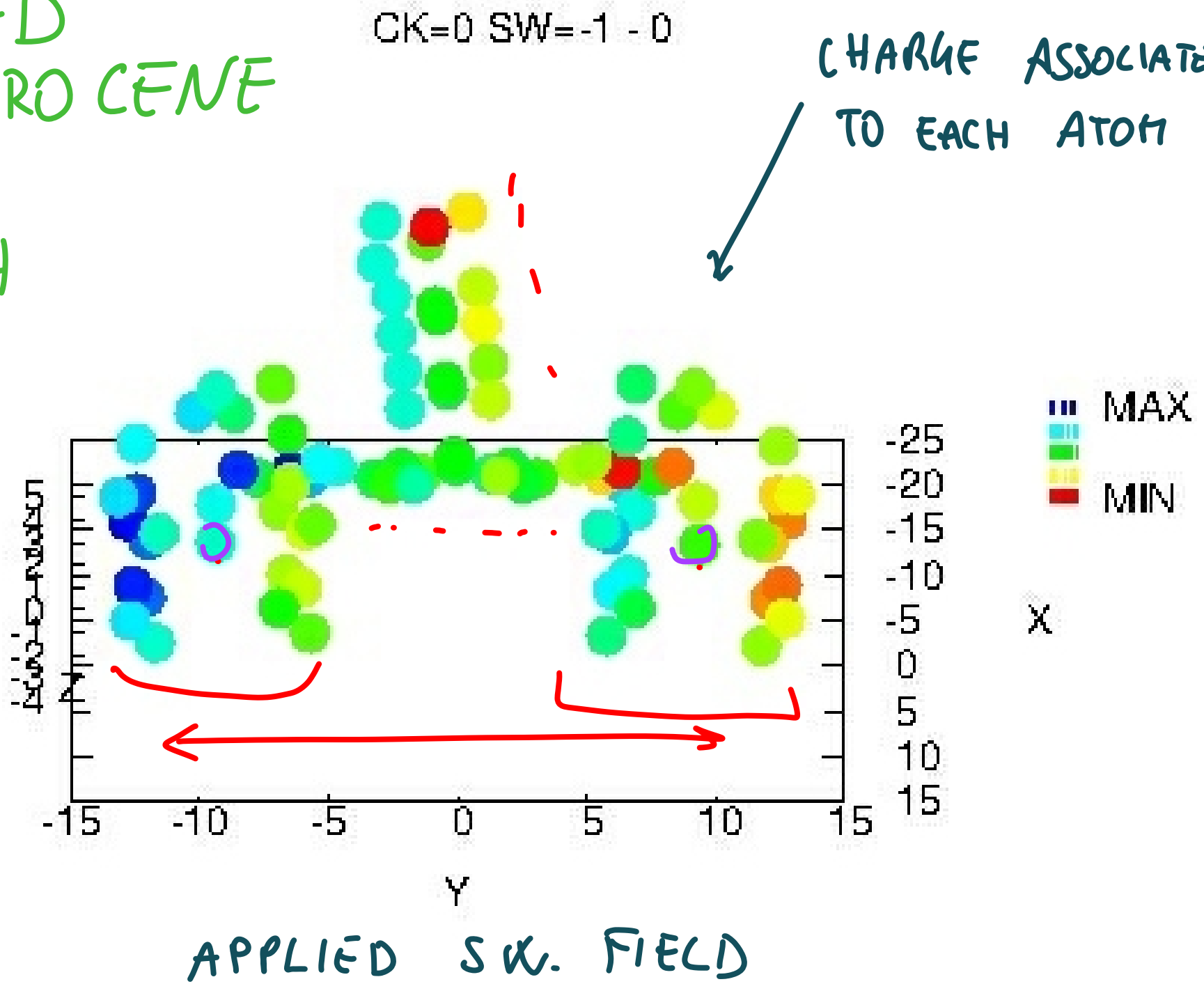
# BISFERROCENE



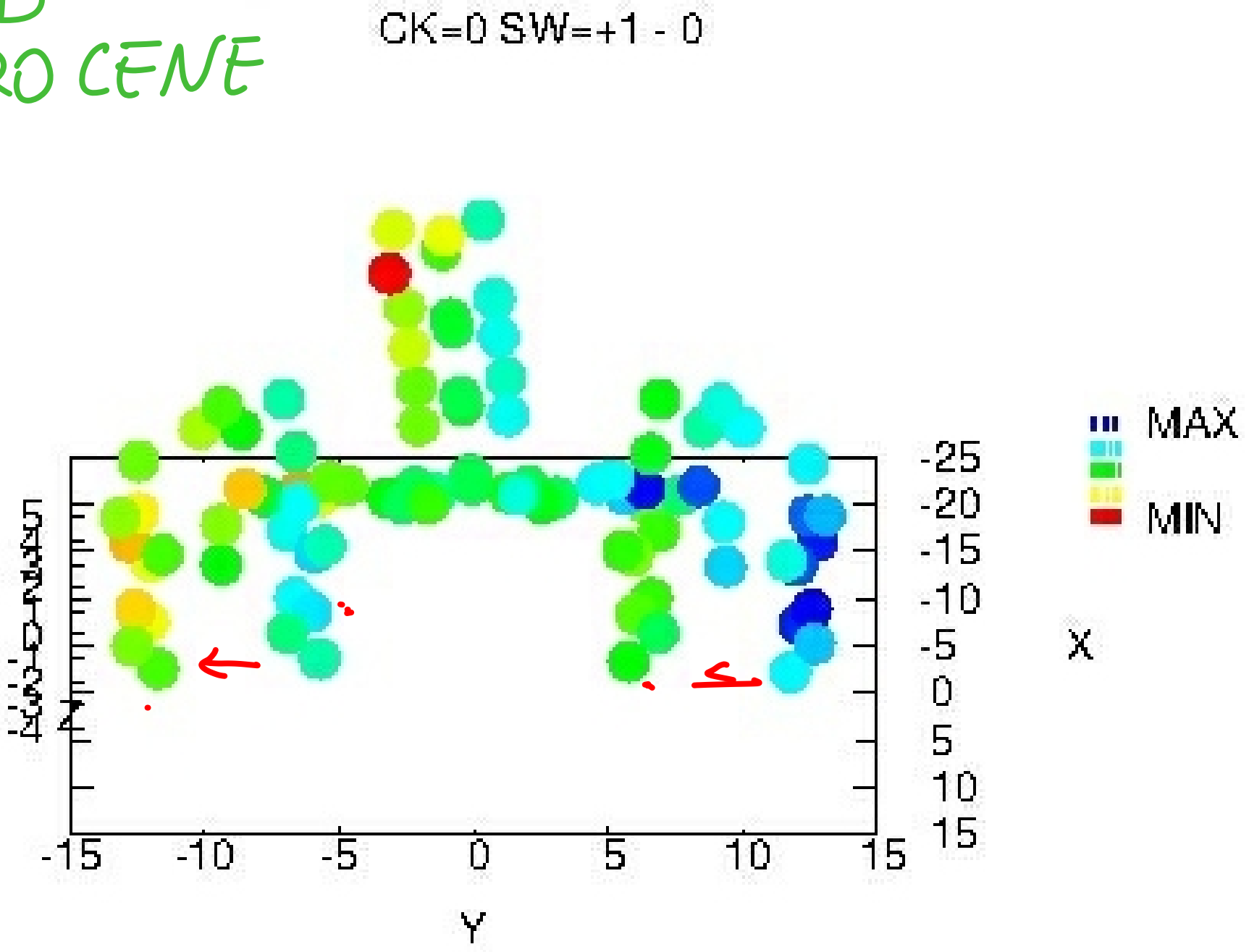

GROUND STATE

HOMO STATE FOR '1' '0'

# TIOLATED BISFERRO CENE UNDER SWITCH E.F.



TIOLATED BISFERRO CENE UNDER SWITCH E.F.




APPLIED IN OPPOSITE DIRECTION

# CRISTALLIZATION

- GENERAL FCN PRINCIPLES
- CLOCKING
- BISFERROCENE AS ELEMENTARY UNIT

# FCN

# Field Coupling Nanocomputing

## Molecular Behavior for FCN

## Model

# MODEL MOLECULAR BEHAVIOR TOWARD FCN APPLICATION

STARTING POINT AB-INITIO SIMULATIONS / REFERENCE POINT

- CPU INTENSIVE
- NO DYNAMIC SIMULATION → MOLECULAR DYNAMICS (FORCE FIELDS)
- NO CONTROL ELECTRODES ← ONLY FORCE E.F. IN A REGION
  EMULATE E.F. WITH POINT CHARGES

⇓

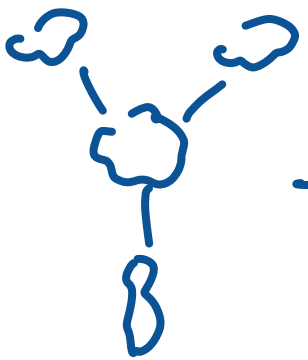
CAN BE USED:

- → CHARACTERIZATION
- → VERIFICATION

} SMALL AMOUNT OF ATOMS

# A NEW APPROACH: 3 STAGES

MOSQUITO



MOLECULE

## I STAGE

AB INITIO SIMULATION CHARACT.

CONDITIONS
- TECH
- INPUT

## II STAGE

POST PROCESSING & GENERATE F.O.M.

CONDITIONS
- TECH
- INPUT
- INTERACTION WITH OTHER ELEMENTS

## III STAGE

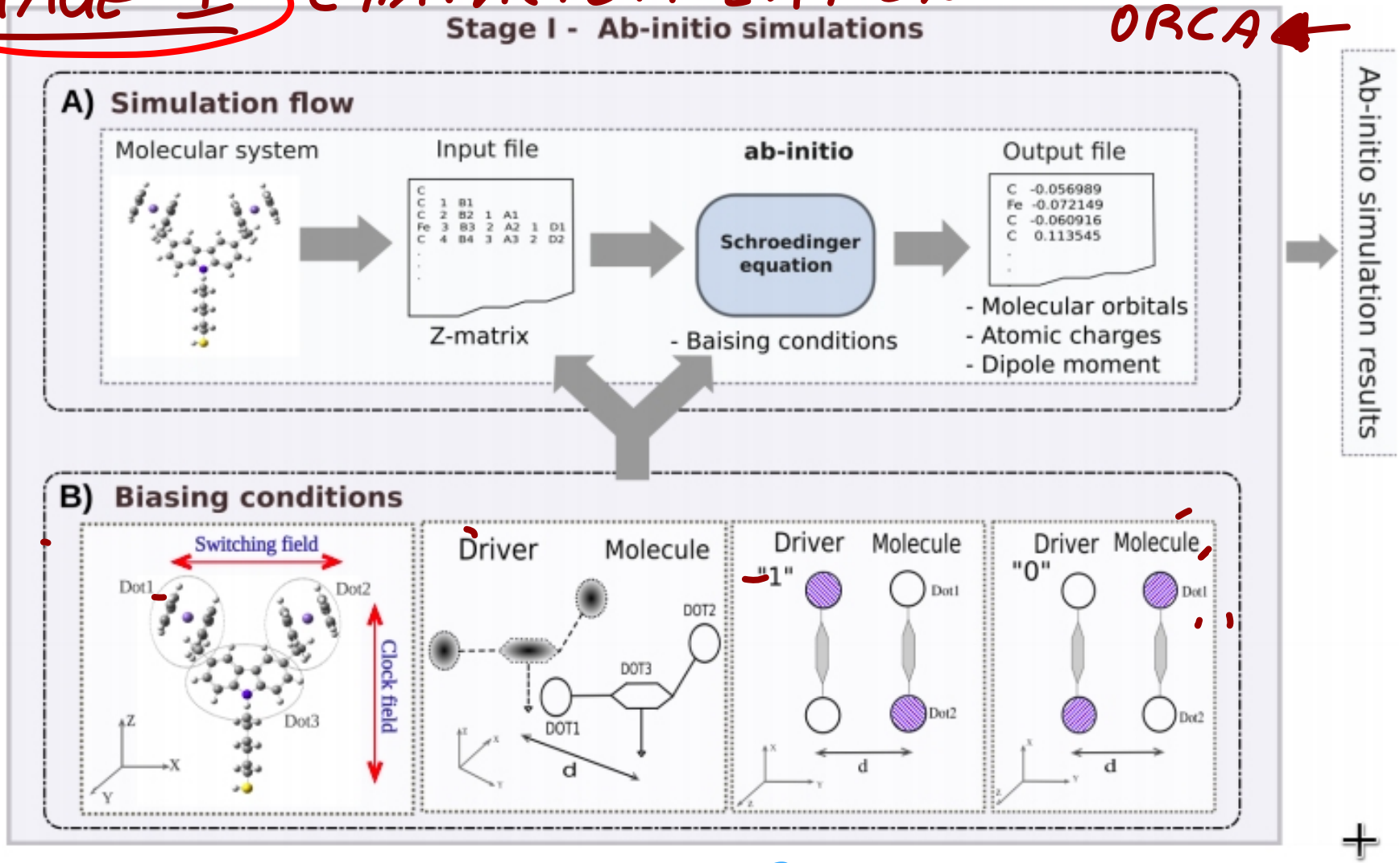
CIRCUIT SIMULATION – ALGORITHM DEVELOP

CONDITIONS
- TECH
- INPUTS
- INTERACTIONS
- CIRCUIT TOPOLOGIES

OBSERVE & STUDY

↳ INFO & FEEDBACK TO TECH

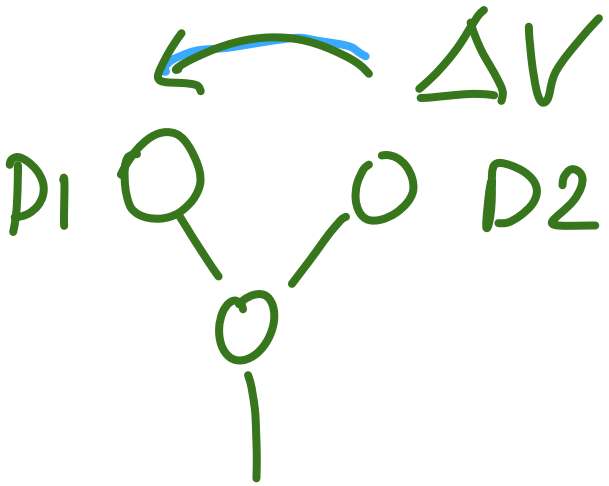
# STAGE I CHARACTERIZATION - GAUSSIAN+ ORCA




- MOL. DESCRIBED USING Z-MATRIX
  - LIST OF ATOMS
  - RELATIVE POSITION (DISTANCES, ANGLES)
- BIASING CONDITIONS
- ITERATIONS ⇒ EXTRACT BEHAVIOR

# CONDITIONS

- INPUT ELECTRIC FIELD

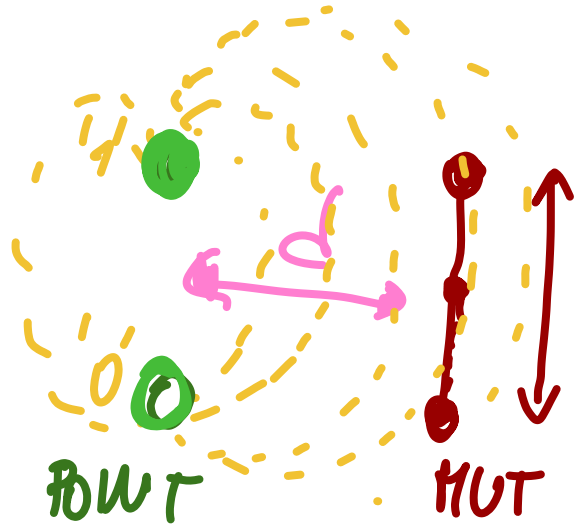



- E.F. BW D1 - D2
- MIN - MAX RANGE

MOLECULE UNDER TEST

# CONDITIONS

- EMULATE THE PRESENCE OF A MOLECULE DRIVER




E.F. GENERATED ACROSS THE 2 DOTS OF MUT

BOWT CHARGES EMULATE DRIVER

CHARACTE-RIZATION } CHANGE THE DISTANCE D
THE RELATIVE VERTICAL POS.
ANGLE TILT

## CONDITIONS

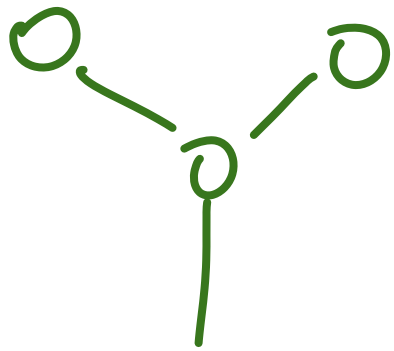
- PRESENCE OF CLOCK

ALL VALUES STORED IN LOOK UP TABLES

DATA RELATET TO
- SINGLE ATOMS
- AGGREGATED BEHAVIOR OF MOLECULE

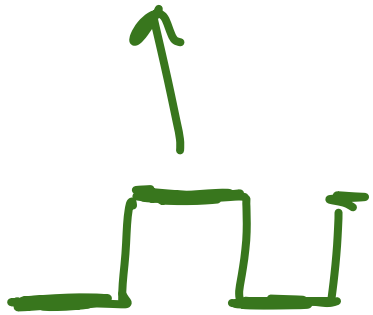
RAW DATA

DUT



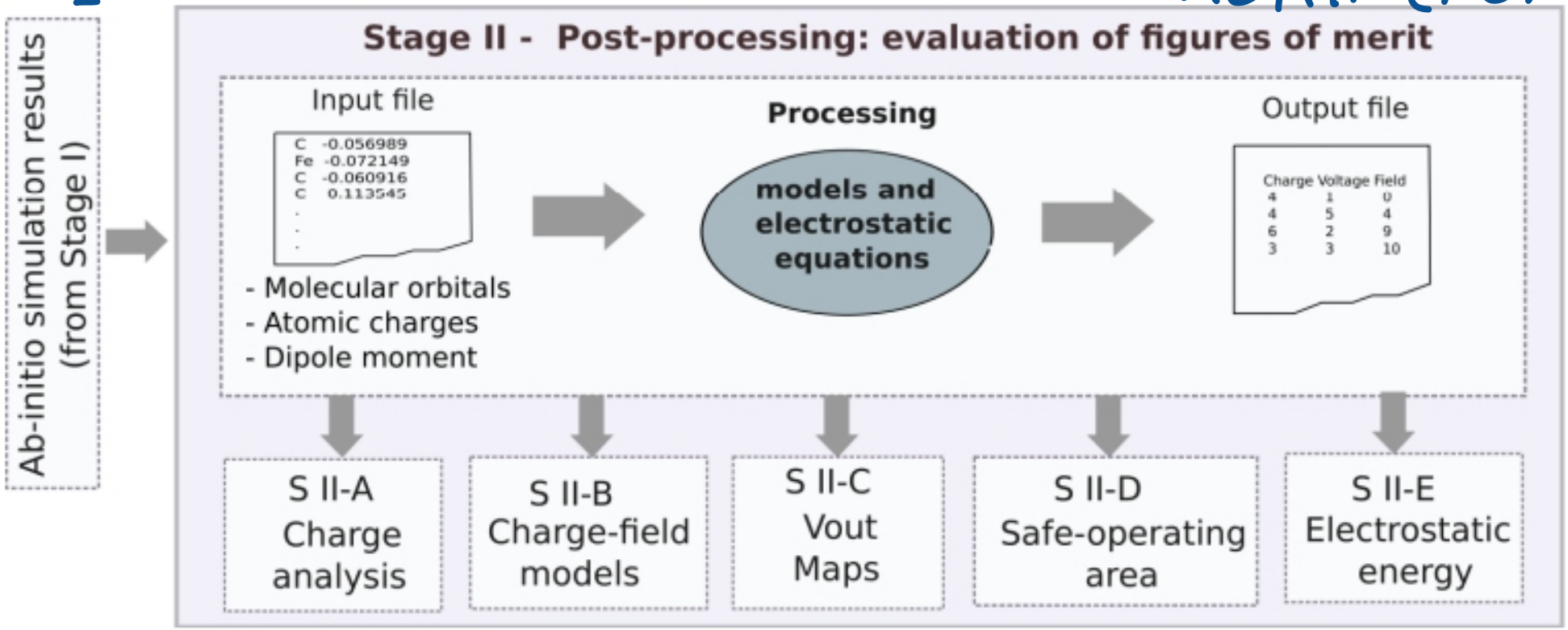
VERTICAL E.F.

- EXPLORE POSSIBLE RANGES
- " TRANSIENT



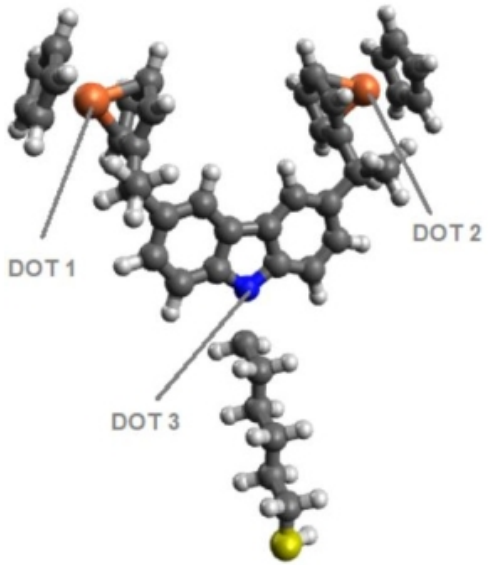
EMULATE TRANSIENT WITH STEP VARIATIONS

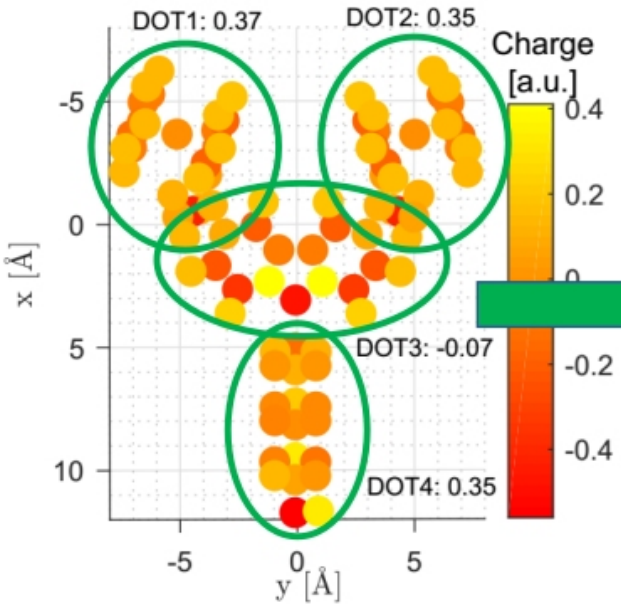
# STAGE II : POST PROCESSING OF RAW DATA → GENERATION OF FIGURE OF MERIT (F.O.M.)

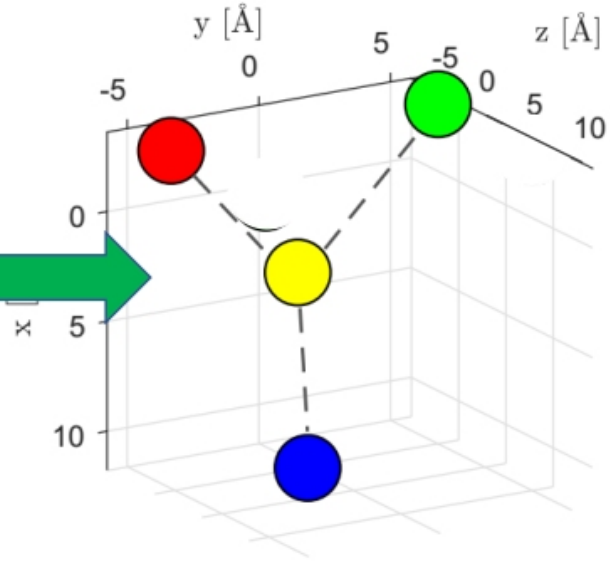



1) AGGREGATED CHARGE ←
2) E.F. GENERATED BY MOL. ←
3) $V_{IN}$ / $V_{OUT}$ CHARACTERISTIC ←

# 1) AGGREGATED CHARGES



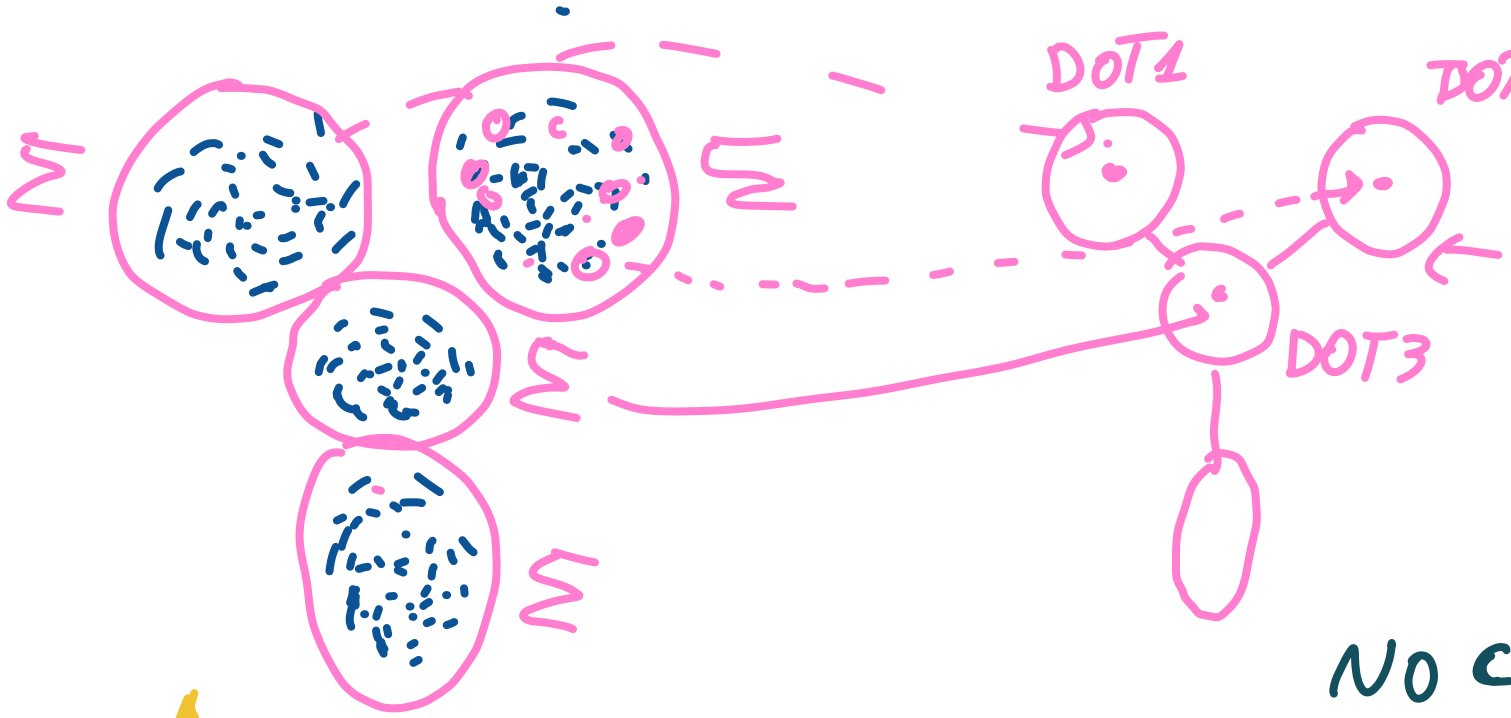




ESP (Electro-Static Potential) charges computed with ab initio software

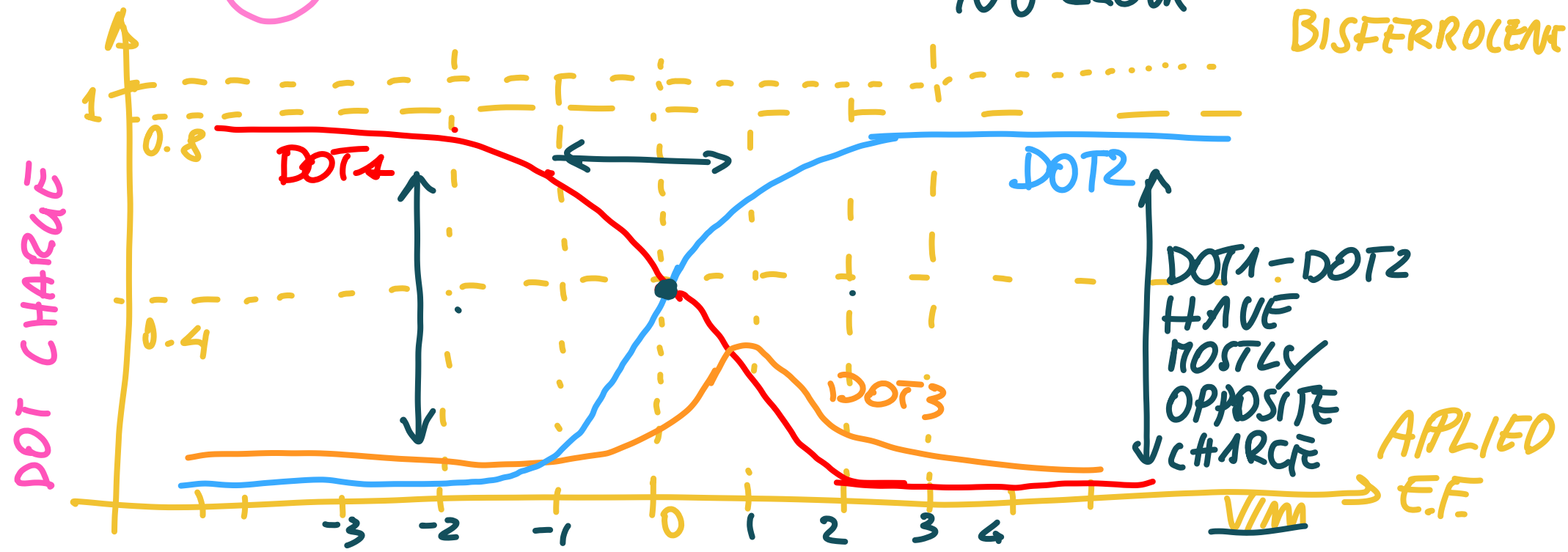
4-charge aggregated charge model
[Pulimeno 2013, Ardesi 2018]

DEMONSTRATION HAS BEEN GIVEN THAT WORKING WITH AGGREGATED VIEW IS EQUIVALENT TO EXTENDED VIEW WITH 81 ATOMS → SAME GENERATED E.F.

# AGGREGATED CHARGE




TOTAL CHARGE ASSOCIATED TO EACH DOT

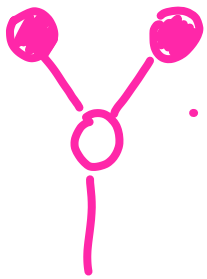


# EFFECT OF CLOCK ON AGGREGATED CHARGE

→ NO INPUT E.F.

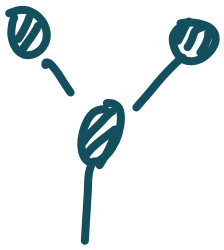
| | DOT1 | DOT2 | DOT3 | |
|---|---|---|---|---|
| A) +2V/m | 0.47 | 0.47 | 0.05 | ACTIVE! |
| B) 0 V/m | 0.37 | 0.35 | 0.27 | ← CHARGE DELOCALIZED |
| C) −2V/m | 0.027 | 0.026 | 0.347 | RESET! |

A)

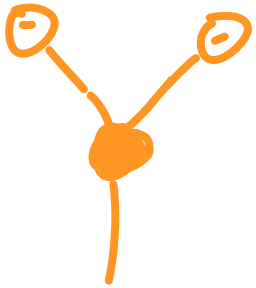


GOOD FOR SWITCH

B)

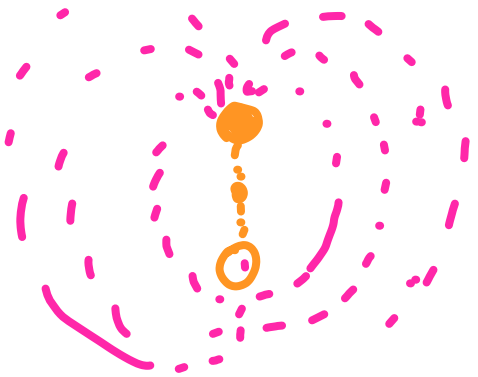


C)



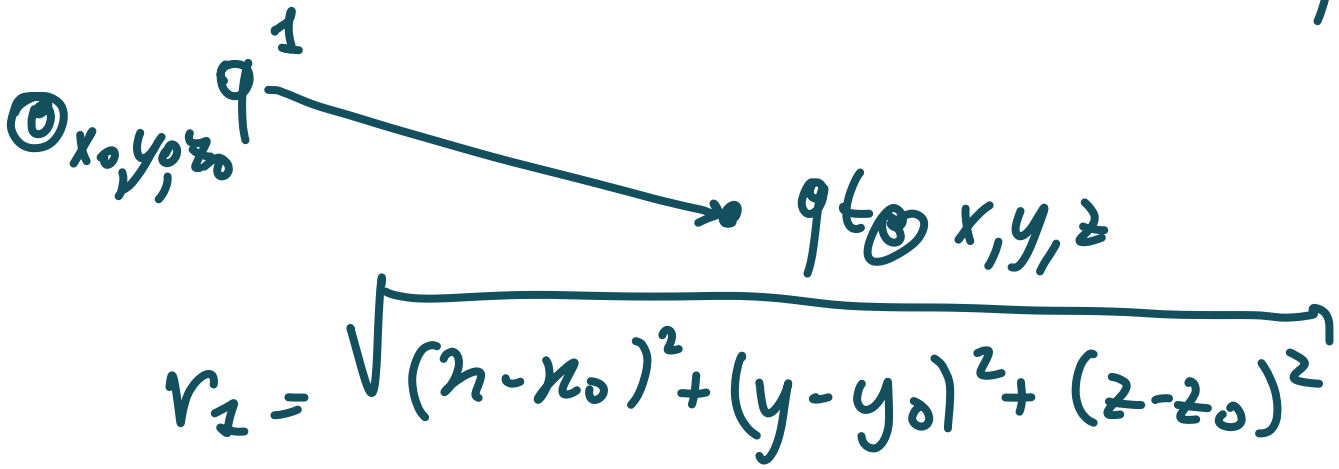
GOOD FOR RESET

# 2) GENERATED E.F. (GENERATED BY A ROC.)

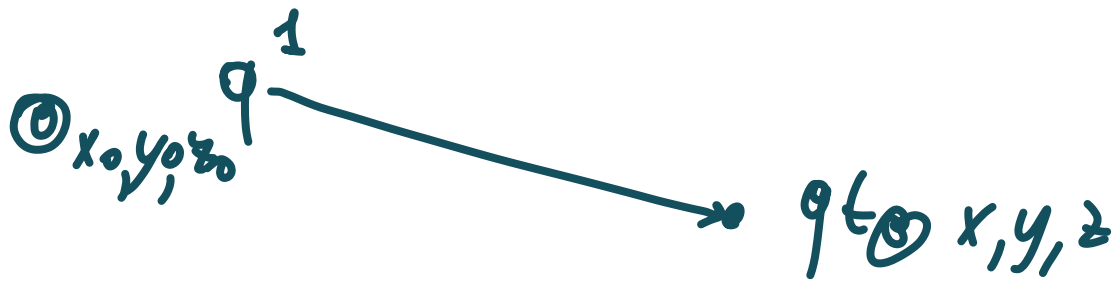


A ROC. WITH A CERTAIN CHARGE DISTR. ⟶ GENERATE E.F. ALL AROUND

IN ORDER TO CALCULATE THE EFFECT ON A P.U.T. FOR NOW LET'S USE A TEST CHARGE $q_t$ IN A GENERIC POINT

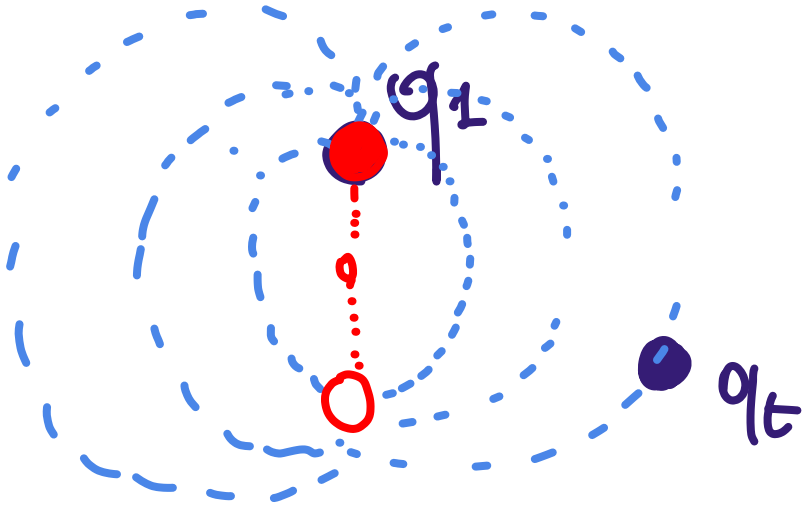



Calculate EF. $E(x, y, z)$ DUE TO $q_1$




APPLY GAUSS' LAW → COULOMB FORCE

$$\vec{F}_1 = \frac{1}{4\pi\varepsilon_0} \cdot \frac{q_1 q_t}{r_1^2} \qquad \vec{E}_1 = \frac{\vec{F}_1}{q_t} = \frac{q_1}{r_1^2} \cdot \frac{1}{4\pi\varepsilon_0} \hat{r}$$



WITH ALL THE MOLECULE CHARGES

$$\vec{F}_{TOT} = \sum_{i=1}^{N} \frac{1}{4\pi\varepsilon_0} \cdot \frac{q_i \cdot q_t}{r_i^2} \hat{r}$$

$$\vec{E}_{TOT} = \frac{\vec{F}_{TOT}}{q_t} = \sum_{i=1}^{N} \frac{1}{4\pi\varepsilon_0} \frac{q_i}{r_i^2} \hat{r}$$

CALCULATED FOR ALL POSSIBLE POINTS IN SPACE WHERE $q_t$ COULD STAY

ACTUALLY RESTRICT IN A VOLUME ←

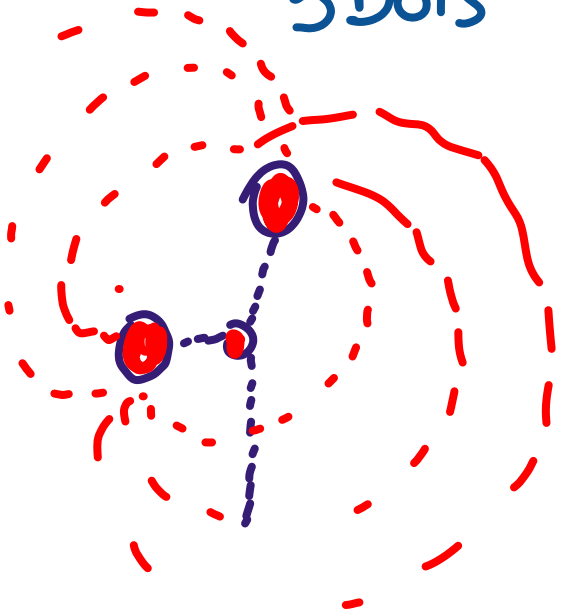
THE GENERATOR $q_i$ CAN BE

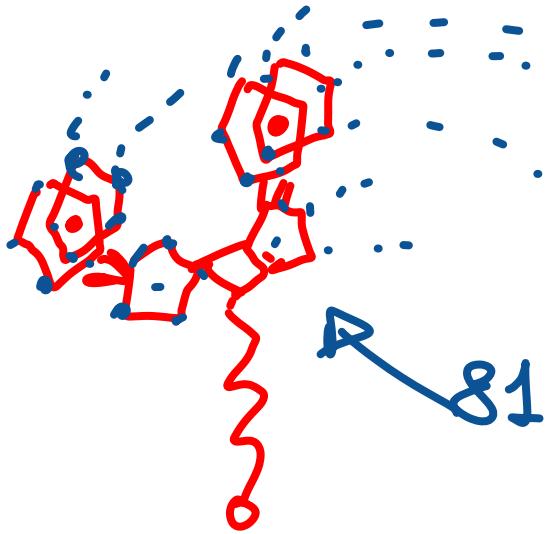
→ $q_i$ OF AGGREGATED CHARGE

→ $q_i$ ASSOCIATETED TO ALL ATOMS IN ROC. (81 atom)

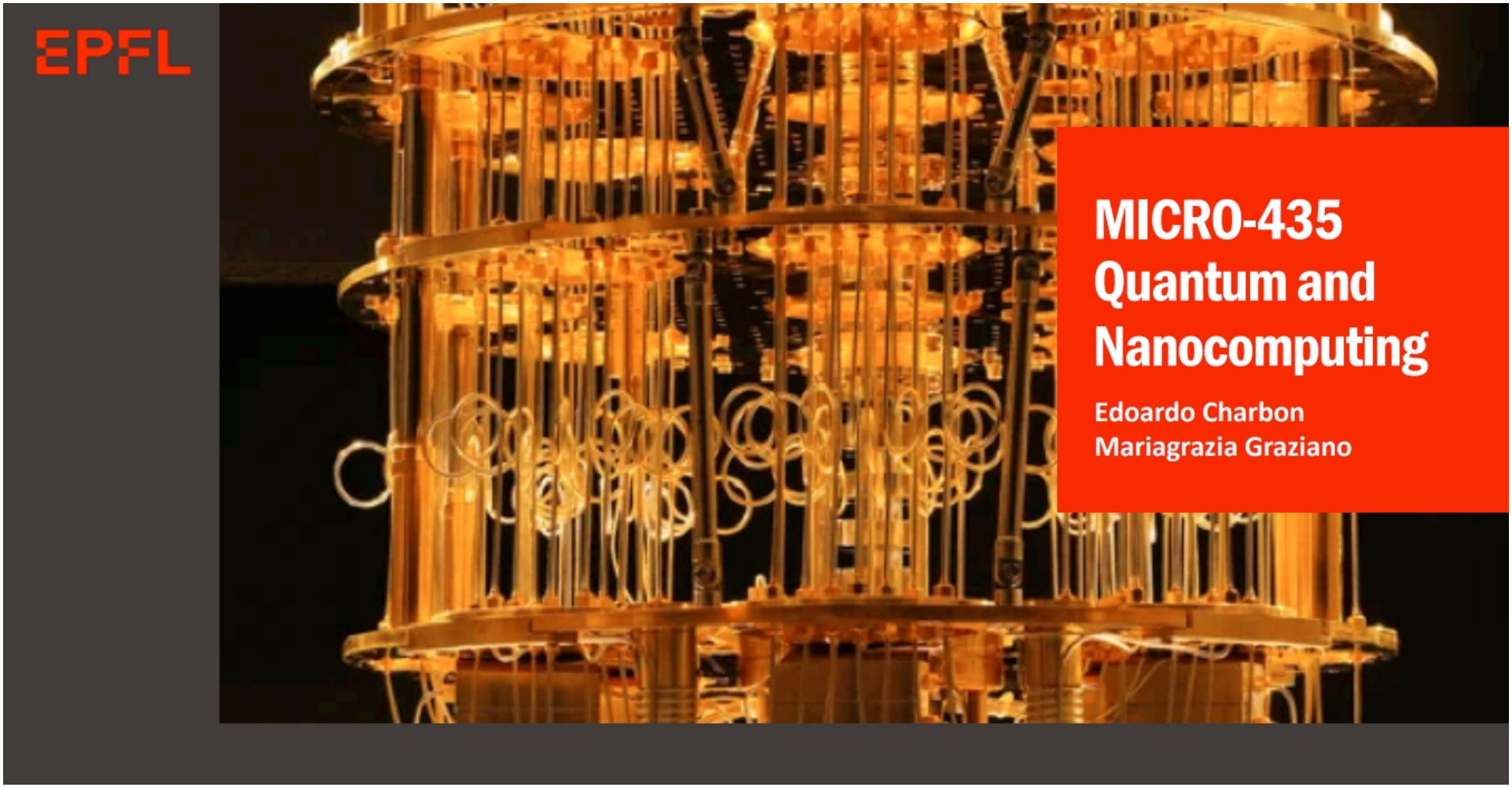
MORE PRECISE ⟶ MORE EXPENSIVE

3 DOTS





81 ATOMS




# MOLECULAR FCN - part 2

# OBJECTIVES

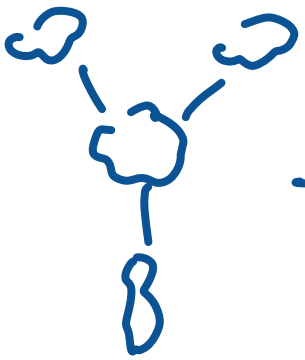
MOLECULAR BEHAVIOR

INTERACTION

SCERPA

# A NEW APPROACH: 3 STAGES

MOSQUITO



MOLECULE

## I STAGE

AB INITIO SIMULATION CHARACT.

CONDITIONS
- TECH
- INPUT

## II STAGE

POST PROCESSING & GENERATE F.O.M.

CONDITIONS
- TECH
- INPUT
- INTERACTION WITH OTHER ELEMENTS

## III STAGE

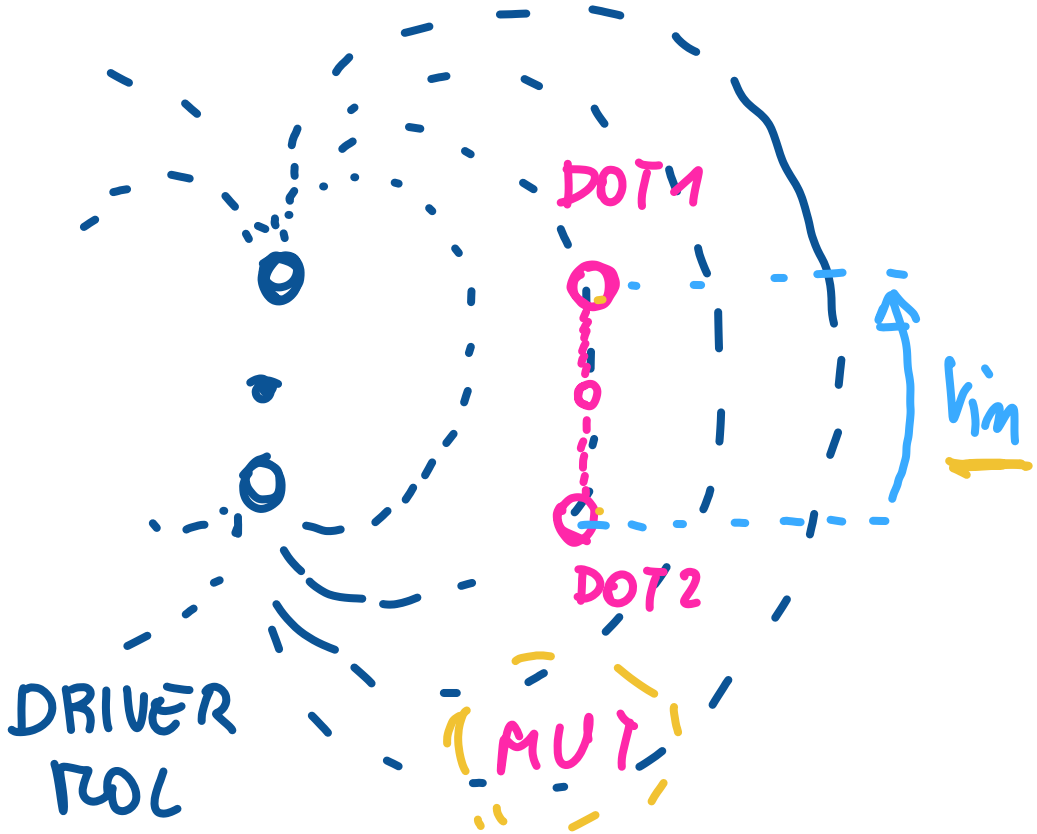
CIRCUIT SIMULATION – ALGORITHM DEVELOP

CONDITIONS
- TECH
- INPUTS
- INTERACTIONS
- CIRCUIT TOPOLOGIES

OBSERVE & STUDY

↳ INFO & FEEDBACK TO TECH

# 3) FROM E.F. TO TRANSCHARACTERISTIC OF MUT




WE ARE INTERESTED IN THE E.F. GENERATED AT MUT SIDE BW D1-D2

A DRIVER GENERATES E.F. AT MUT LOCATION

⇓

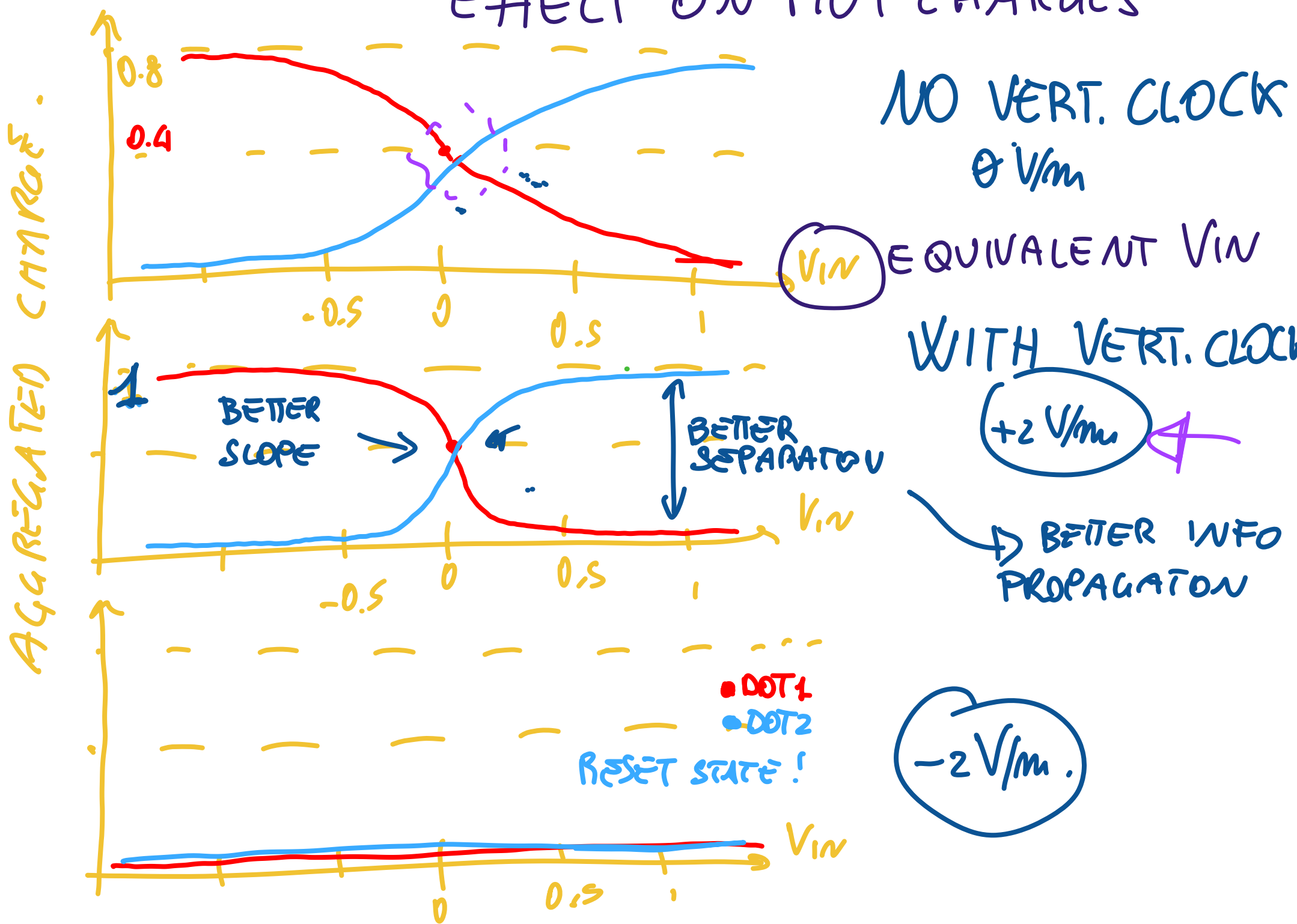
CALCULATE EQUIVALENT Vim AT MUT SITE

(INTEGRAL OF E.F.)

↓ W/ ↓ WOUT

REPEATED → CLOCK AT THE DRIVER

# EFFECT ON MUT CHARGES




NO VERT. CLOCK

0 V/m

EQUIVALENT VIN

WITH VERT. CLOCK

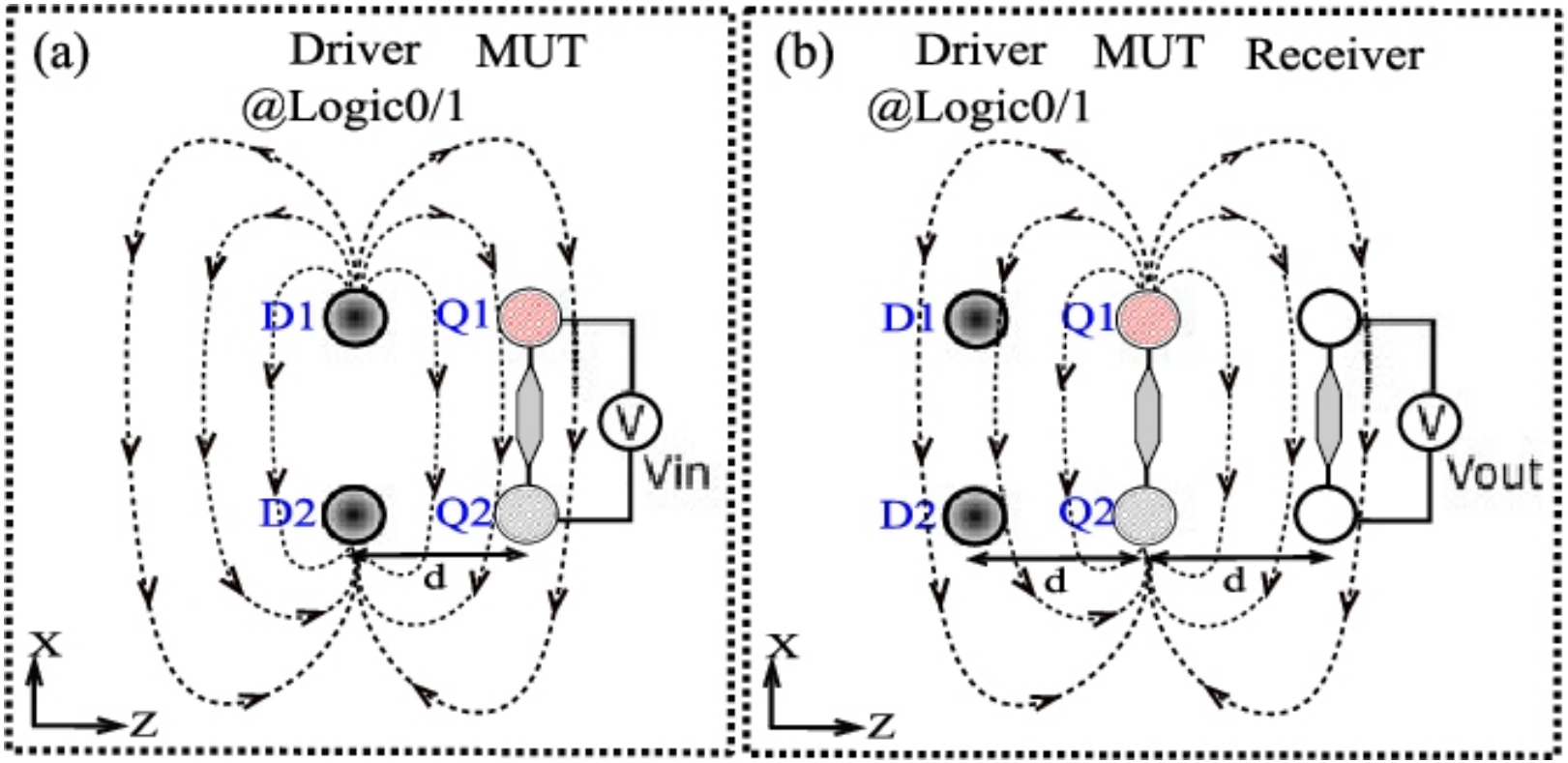
+2 V/m

BETTER INFO PROPAGATION

-2 V/m.

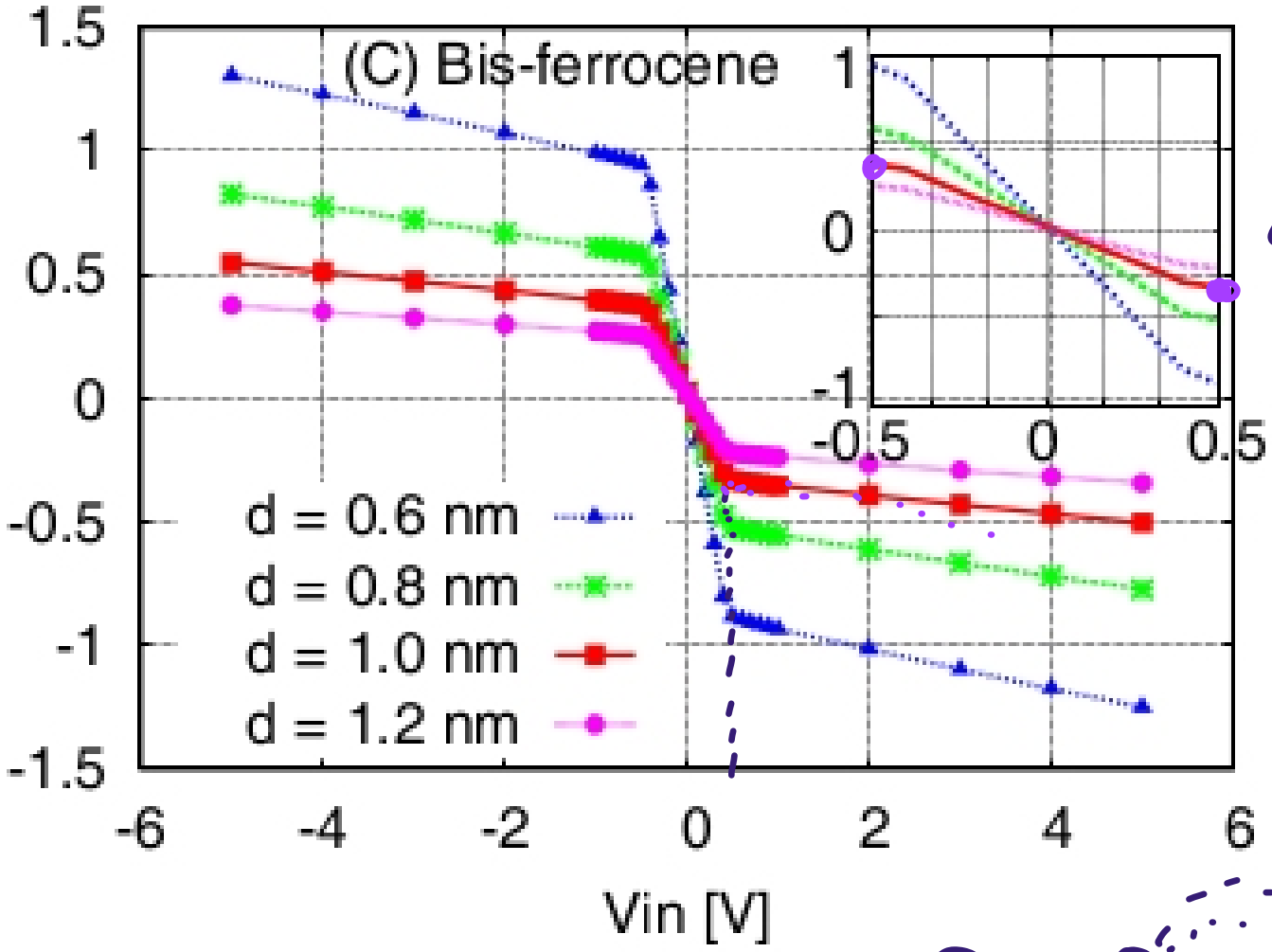
SEE THE EFFECT ON A RECEIVER

$V_{IM}$ — $V_{ONT}$ TRANCHARACTERISTIC



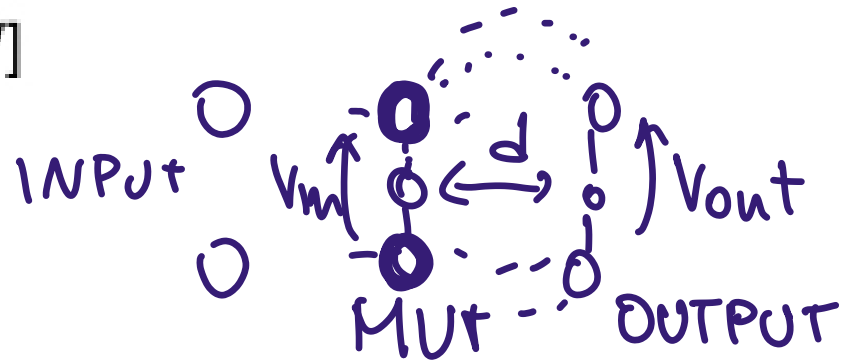

PREVIOUS PICTURE

# TRANSCHARACTERISTICS FOR VARIOUS DISTANCES OF MUT

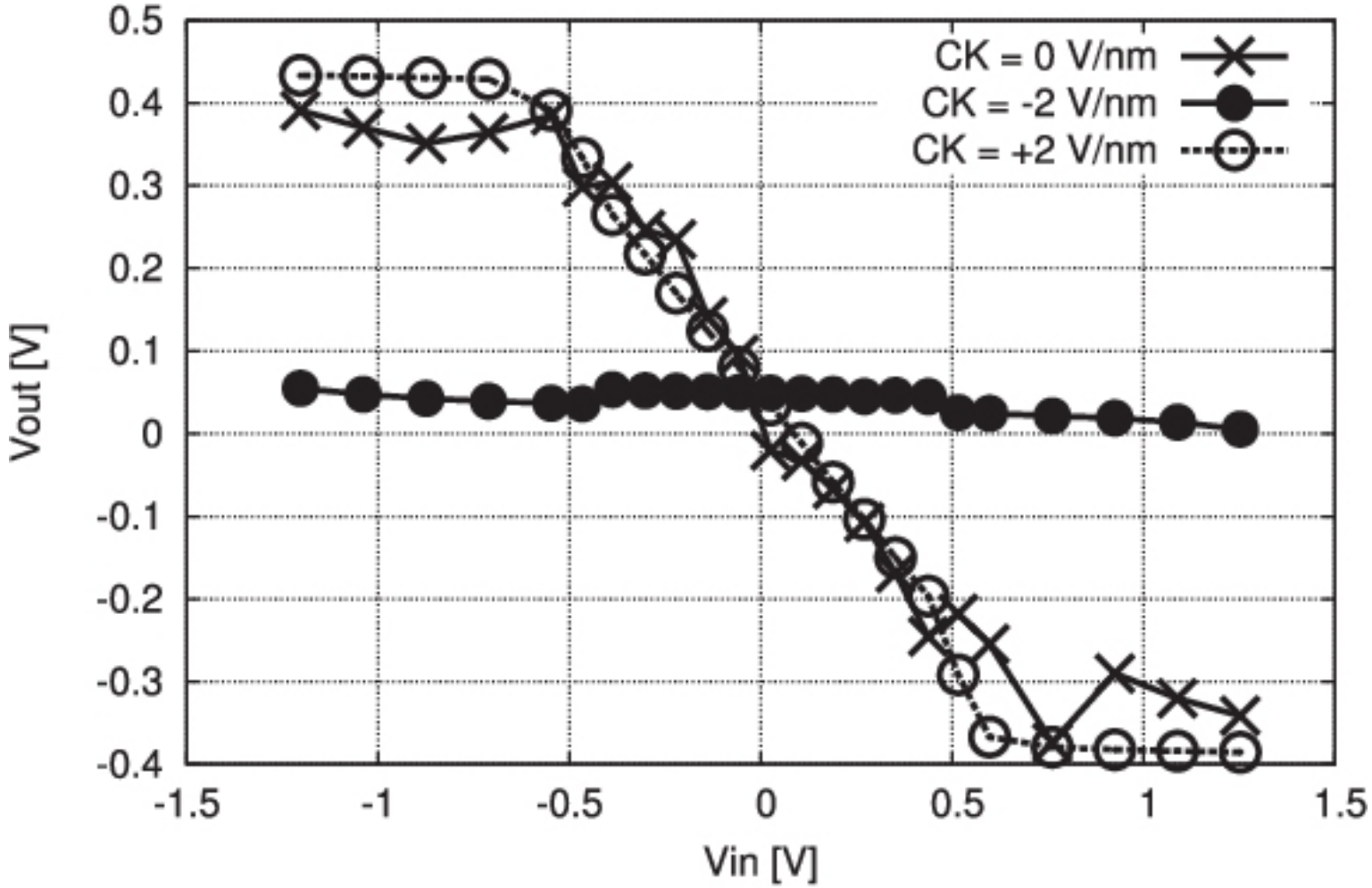



d = 1nm
LOSS!

d = 0.8m
OK!



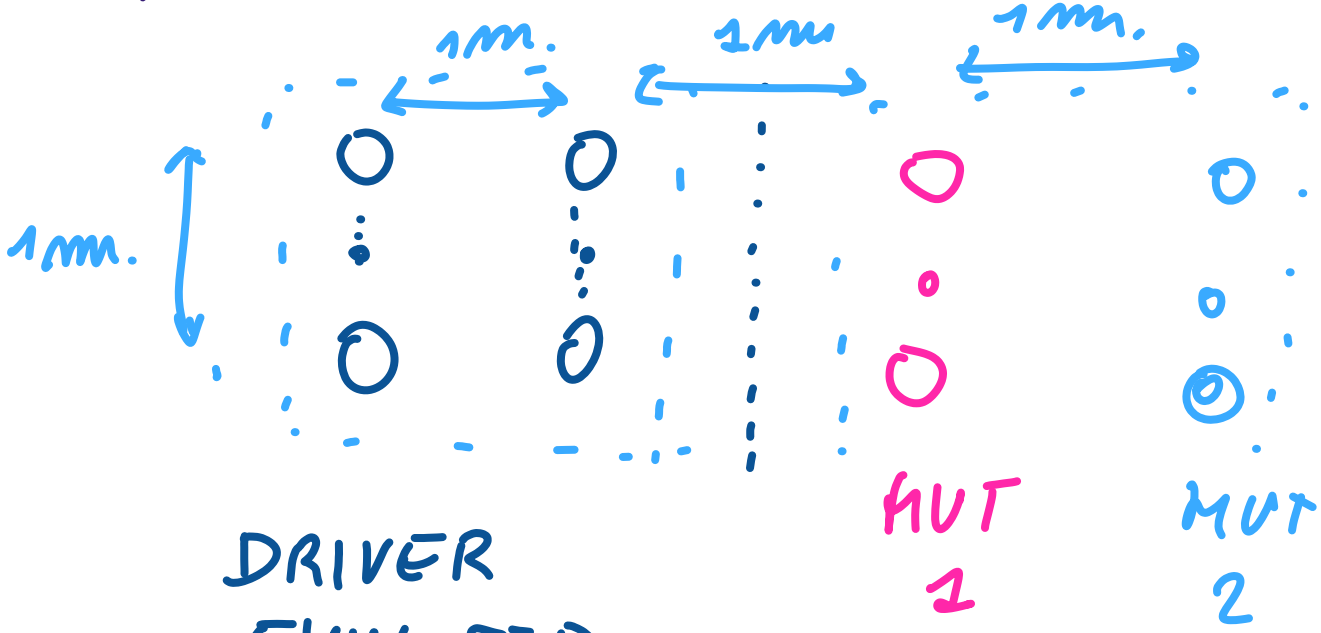
# IMPACTO OF CLOCK ON Vout/Vin @ 1 nm

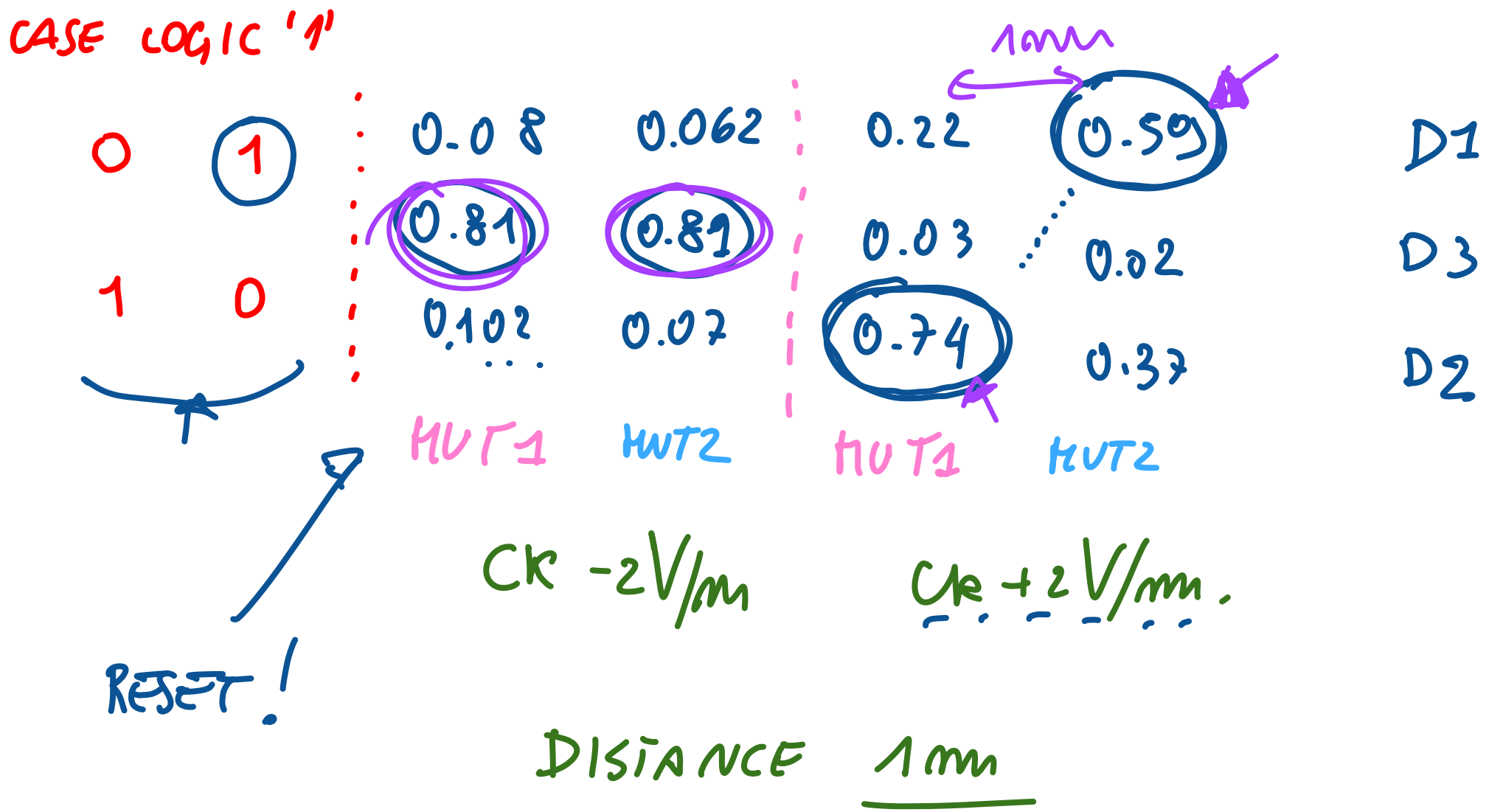


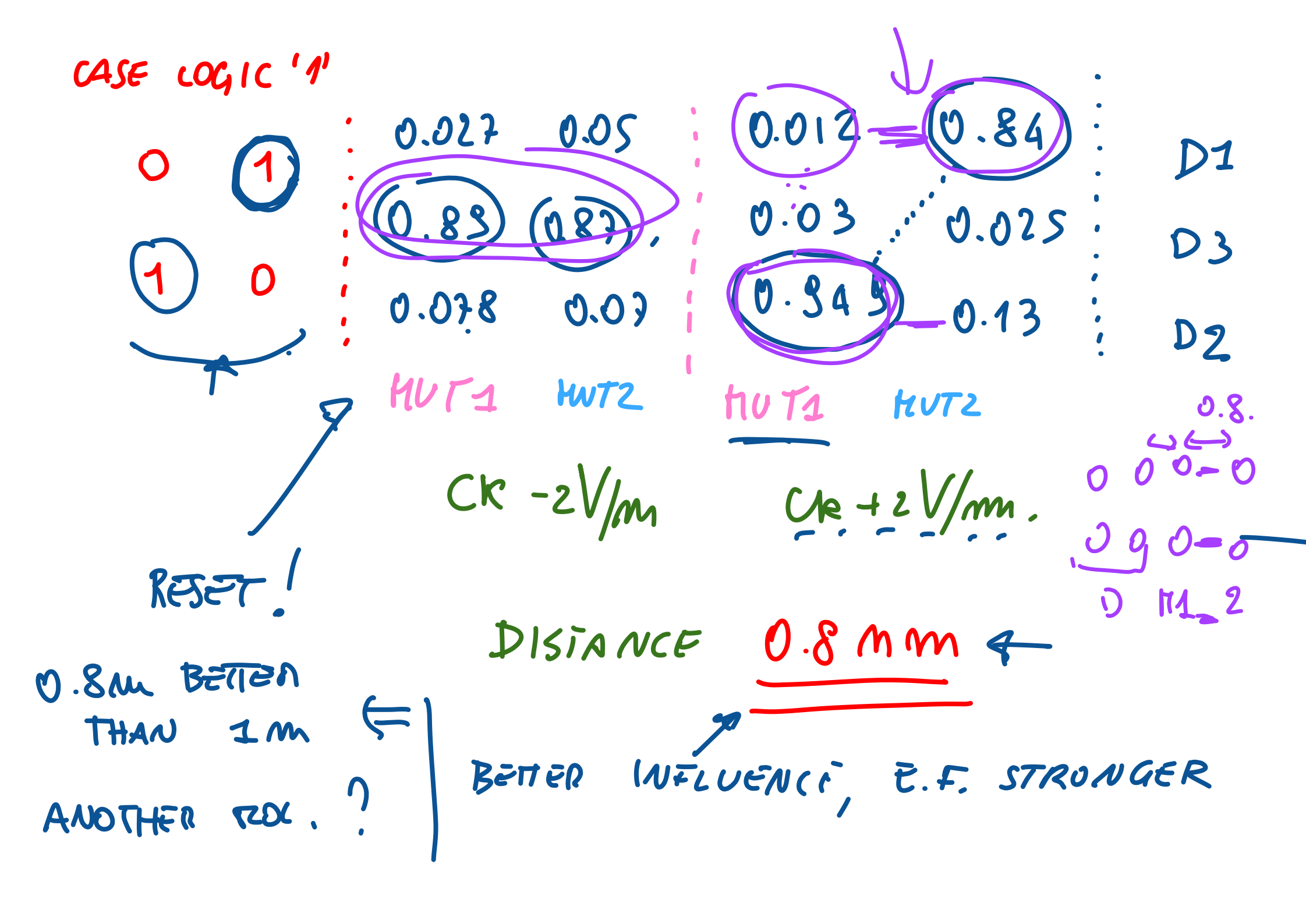

(a)

# STAGE III: TOWARD A MODEL OF INTERACTION AMONG MANY MOLECULES

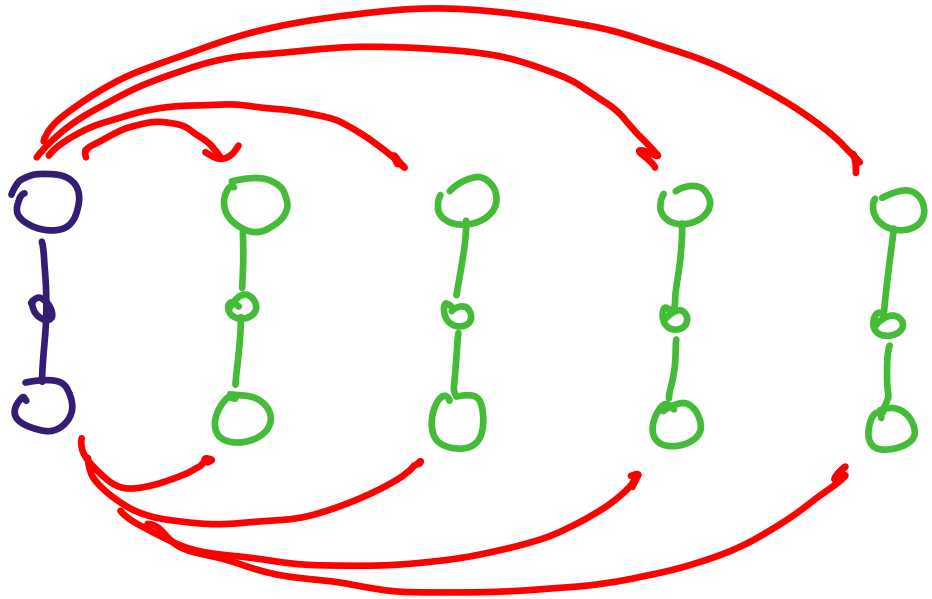
## III.a) FIRST REFERENCE POINT: AB-INITIO SIM



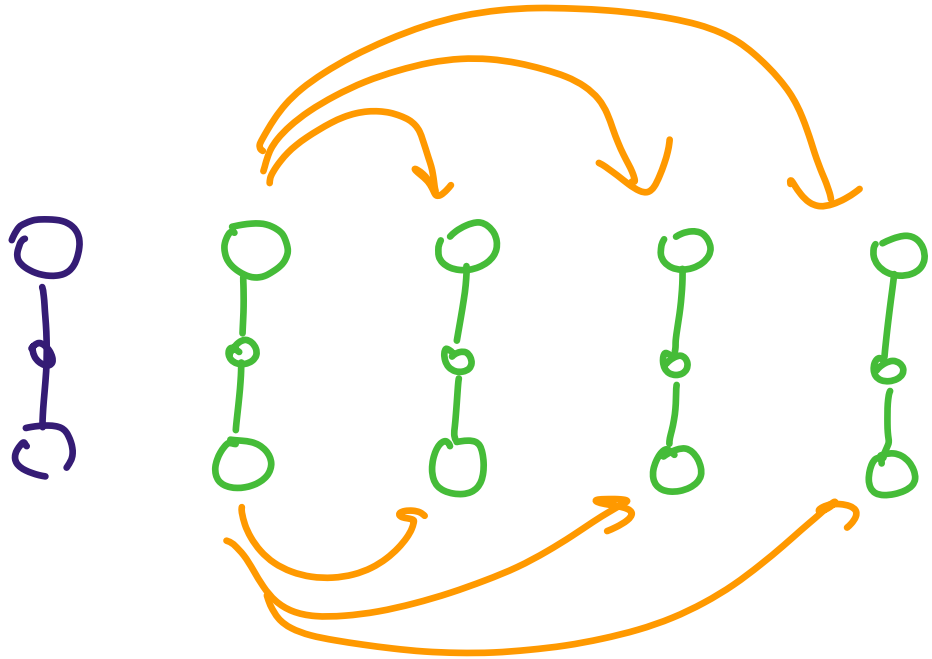

CASE LOGIC '1'
0
1
1
0
RESET !
0.08
0.062
0.81
0.81
0.102
0.07
HUT1
HUT2
1mm
0.22
0.59
0.03
0.02
0.74
0.37
HUT1
HUT2
D1
D3
D2
CK -2V/m
Ck +2V/m.
DISTANCE 1mm


CASE LOGIC '1'
0
1
1
0
0.027
0.05
0.83
0.87
0.078
0.07
HUT1
HUT2
0.012
0.84
0.03
0.025
0.845
0.13
HUT1
HUT2
D1
D3
D2
0.8.
D M1 2
CK -2V/m
CK +2V/m.
RESET!
DISTANCE
0.8 mm
0.8m BETTER THAN 1m
ANOTHER REX. ?
BETTER INFLUENCE, E.F. STRONGER

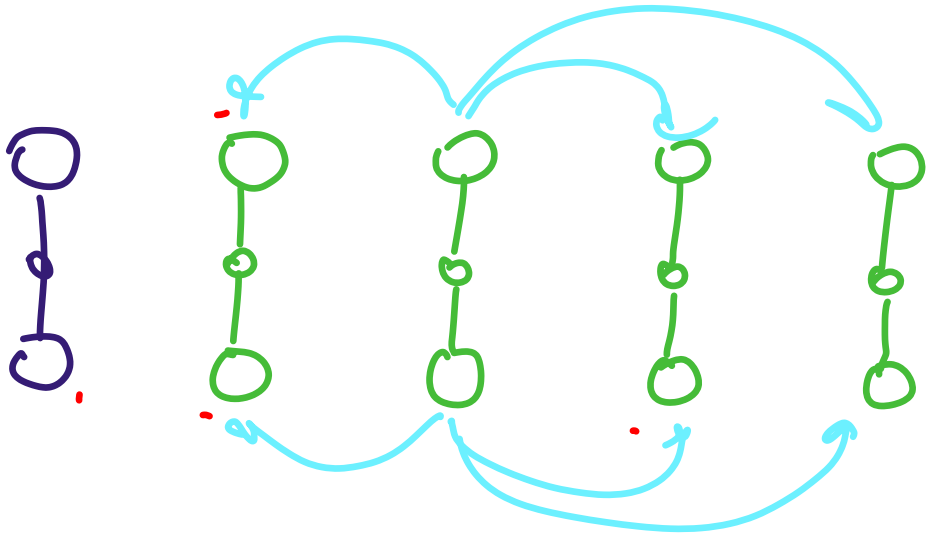
# PHASE III. b) INFO PROPAGATION TO CIRCUIT



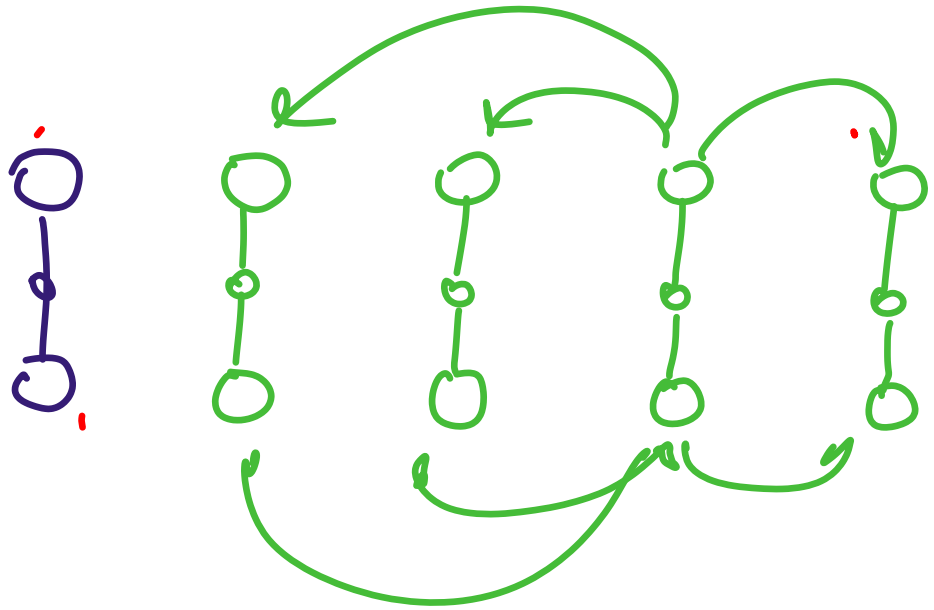
# PHASE III. b) INFO PROPAGATION TO CIRCUIT



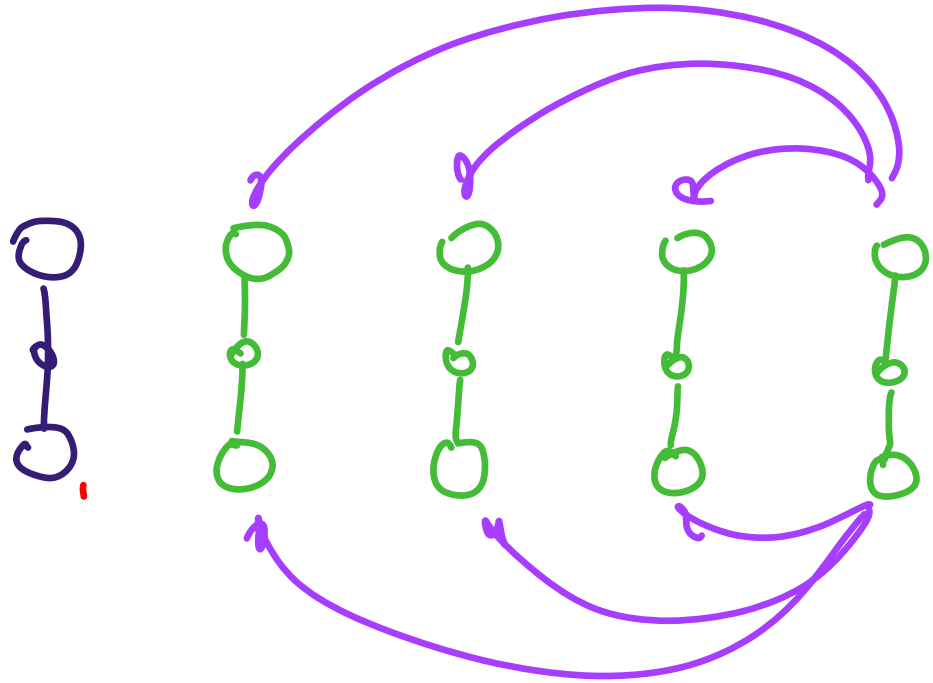
# PHASE III. b) INFO PROPAGATION TO CIRCUIT



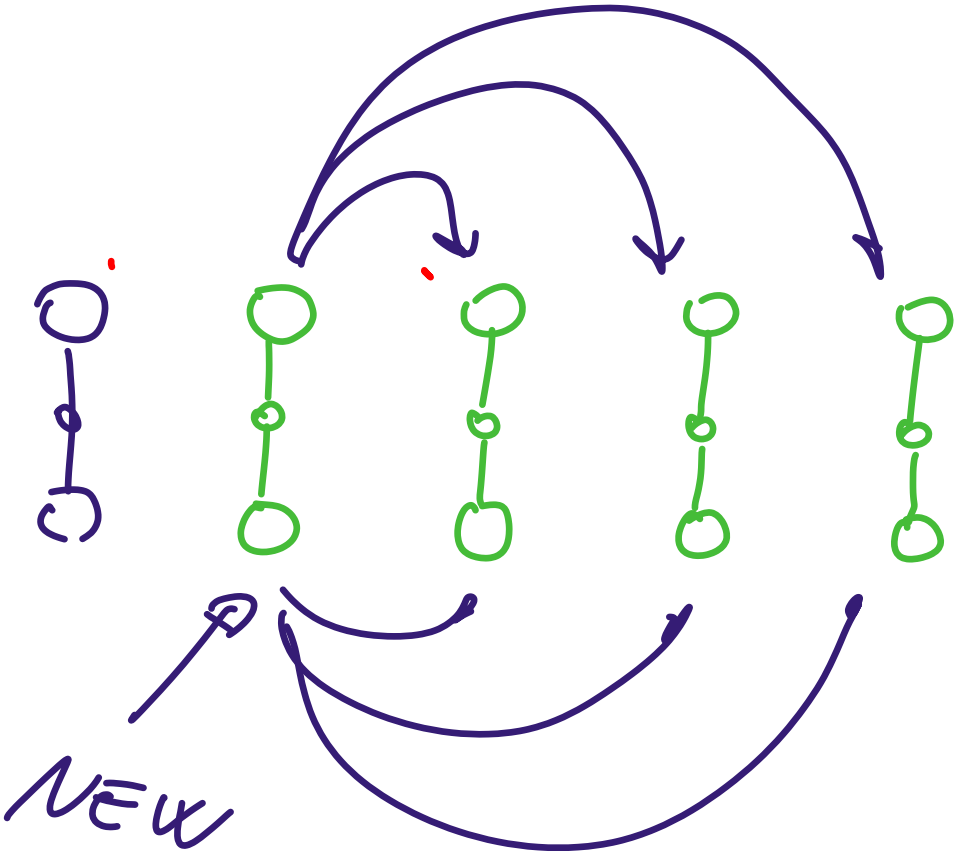
# PHASE III. b) INFO PROPAGATION TO CIRCUIT



# PHASE III. b) INFO PROPAGATION TO CIRCUIT



# PHASE III. b) INFO PROPAGATION TO CIRCUIT



NEW FIELD DUE TO ALL DRIVERS!

EACH Π. IS A

→ RX
→ TX

} ANTENNA

# PHASE III .b) INFO PROPAGATION TO CIRCUIT

USE THE TRANSCHARACTERISTIC

$\forall MOL_i$

$Q_{1i}(E_{CK}, V_{im_i}^{TOT})$

$Q_{2i}(E_{CK}, V_{im_i}^{TOT})$

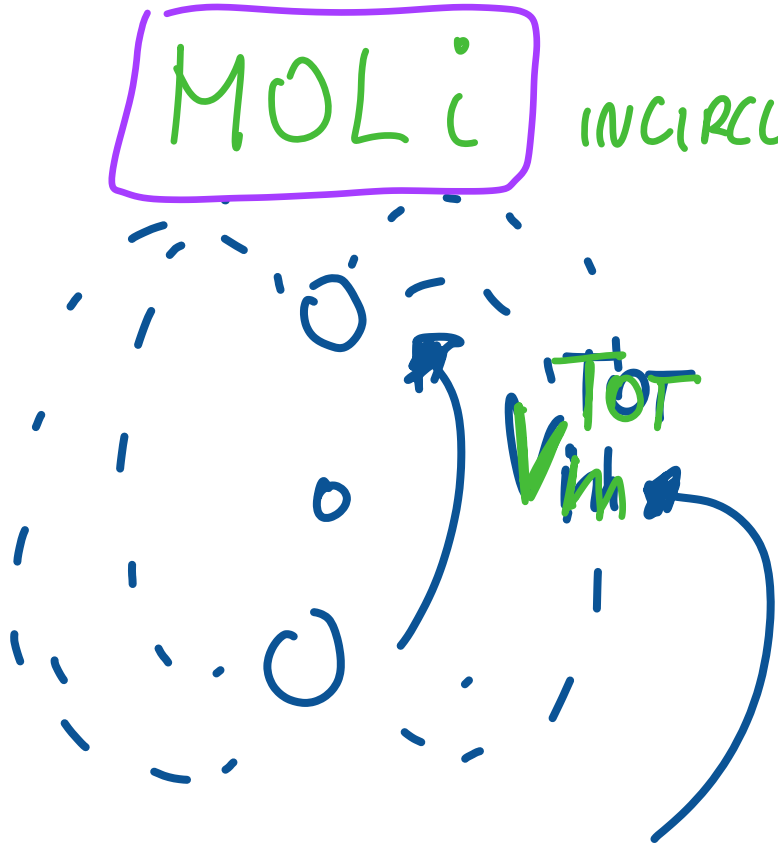
$Q_{3i}(E_{CK}, V_{im_i}^{TOT})$

STORED IN L.U.T. AFTER PHASE I, PHASE II

$\Rightarrow$

DATA CAN BE STORED → 3DOTS MODEL

→ ALL 81 ATOMS




DUE TO ALL POSSIBLE SOURCES

# EQUIVALENT INPUT VOLTAGE

$$V_{im,i}^{TOT} = V_{im,i}^{DRIVER} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \left[ V_{im,i}^{Q_{1j}} + V_{im,i}^{Q_{2j}} + V_{im,i}^{Q_{3j}} \right]$$

EQUIVAL. INPUTVOLTAGE AT MOL. i DUE TO DOTS WITH Q1 OF MOL. j.

IN A CIRCUIT, GIVEN A DRIVER CONF. WE WANT TO KNOW

$$\forall \text{MOS}\, i \quad Q_{1i};\ Q_{2i};\ Q_{3i}$$

REMINDER: ALL MOSs INFLUENCE EACH OTHER

- CANNOT BE SOLVED LINEARLY
- ITERATIVE SELF CONSISTENT SOLUTION
- WE NEED TO REACH A CONVERGENCY $\varepsilon$


GIVEN A CIRCUIT:

DRIVER CONFIG.

N° OF MOLECULES

LAYOUT

ALGORITHM.

1. INITIALIZATION
2. SELF-CONSISTENT LOOP CALCULATE INTERACTION
3. EVALUATE FINAL CHARGE DISTRIBUTION

(1) INIT.
- MOL. POSITION (LAYOUT)
- INITIAL CHARGE $\rho_{mol}$
- DRIVER CONF
- CK CONF.

↖ AT THE MOMENT TO NO CK. PHASES

→ DAFTER EXTEND TO CK PH.

(2) MOL-INTERACTION

- $\forall$ MOL $i$ CALCULATE EFFECT OF $D$ ( $D \rightarrow EF_{@MI}$ , $\rightarrow V^{D}_{im,i}$ )

$$\forall_i \quad V_{im,i} = V^{D}_{im\,i}$$

- WHILE ERROR $< \varepsilon$ DO
  - $\forall i$ DO
    - EVALUATE $Q_{1i}$, $Q_{2i}$, $Q_{3i}$ ← TRANSCAR.
    - $\forall$ MOL $j \neq i$ DO EVALUAT. $\Delta V_{MOL\,j\text{-}TO\text{-}MOL\,i}$; STORE it
  - EVALUATE MAXIMUM TOTAL VOLTAGE VARIATION $\Delta V$ AMONG ALL COUPLE $j$-$i$ : ERROR ...

$\Delta V_{MOL\,j\text{-}TO\text{-}MOL\,i}$ :

AT EACH STEP OF THE LOOP THE CHARGE OF MOL $j$ CHANGES OF $\Delta Q_1, \Delta Q_2, \Delta Q_3$ DUE TO OTHER MOL. → COMPUTE $\Delta V$

$$\Delta V_{MOL\,j\text{-}TO\text{-}MOL\,i} = \Delta V_{IM,i}^{\Delta Q_{1,j}} + \Delta V_{IM,i}^{\Delta Q_{2,j}} + \Delta V_{IM,i}^{\Delta Q_{3,j}}$$

3

# FINAL EVALUATION

FOR $V_{im,i}$ CALCULATE $\forall_i$

$\Downarrow$

$Q_{1,i}, Q_{2,i}, Q_{3,i}$

USING CHARACTERISTIC

# THE ALGORITHM IN SHORT

WHILE CONVERGENCY REACHED

$\forall$ vol i

$\forall$ vol j : $\Delta v_{j \to i}$

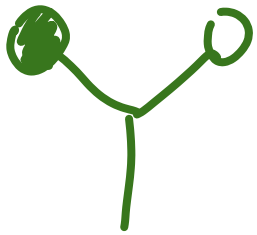
ADDENDUM: in case i ↗↗ (j ↗↗)

very distant vol have negligible influence

→ a certain R RADIUS OF INFLUENCE CAN BE DEFINE TO REDUCE COMP. EFFORT

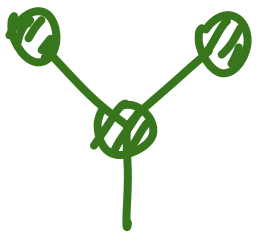
# STABILITY

if MOL. ALONE



INPUT FORCE

CHARGE IS LOCALIZED



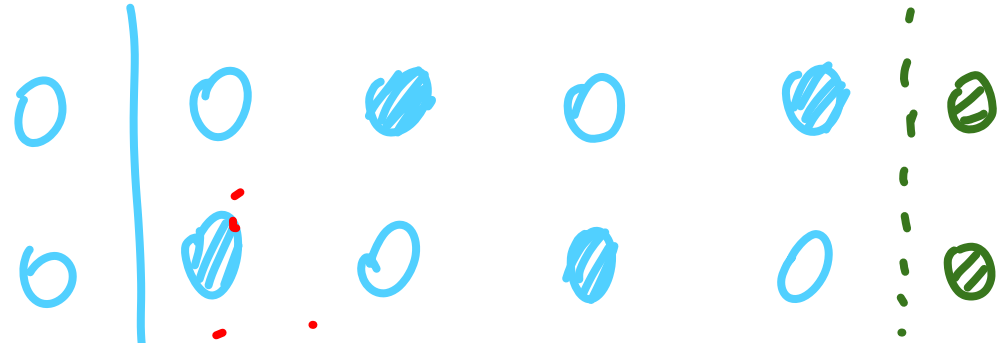
INPUT IS RELEASED

CHARGE IS DELOCALIZED

MOLECULE IS NOT BISTABLE

if MOL IN WIRE

IT BECOMES BISTABLE

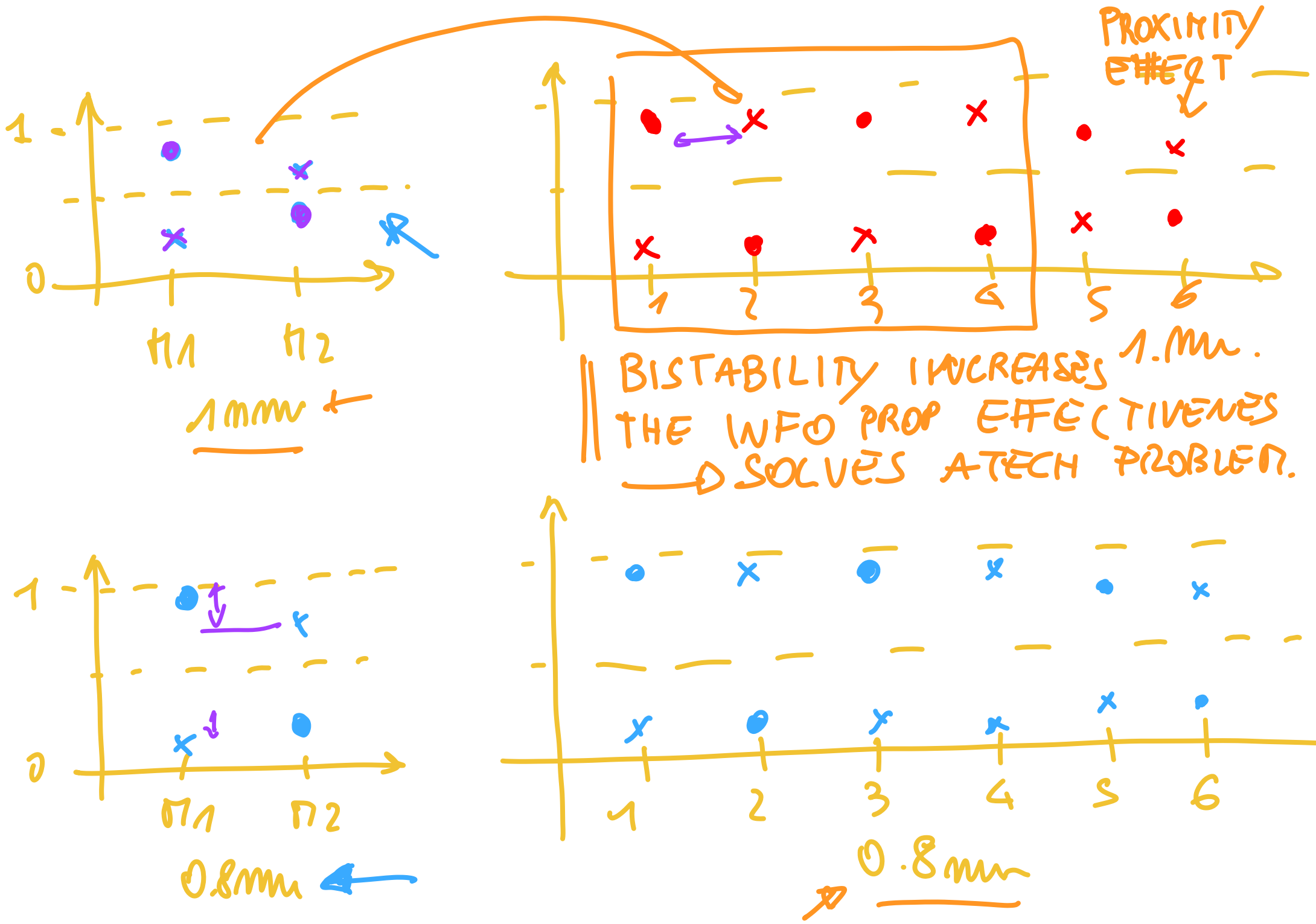


DRIVER RELEASED

AFTER THE PROP. STARTED FROM DRIVER

→ CHARGES IN WIRE REMAIN STABLE EVEN DRIVER RELEASE

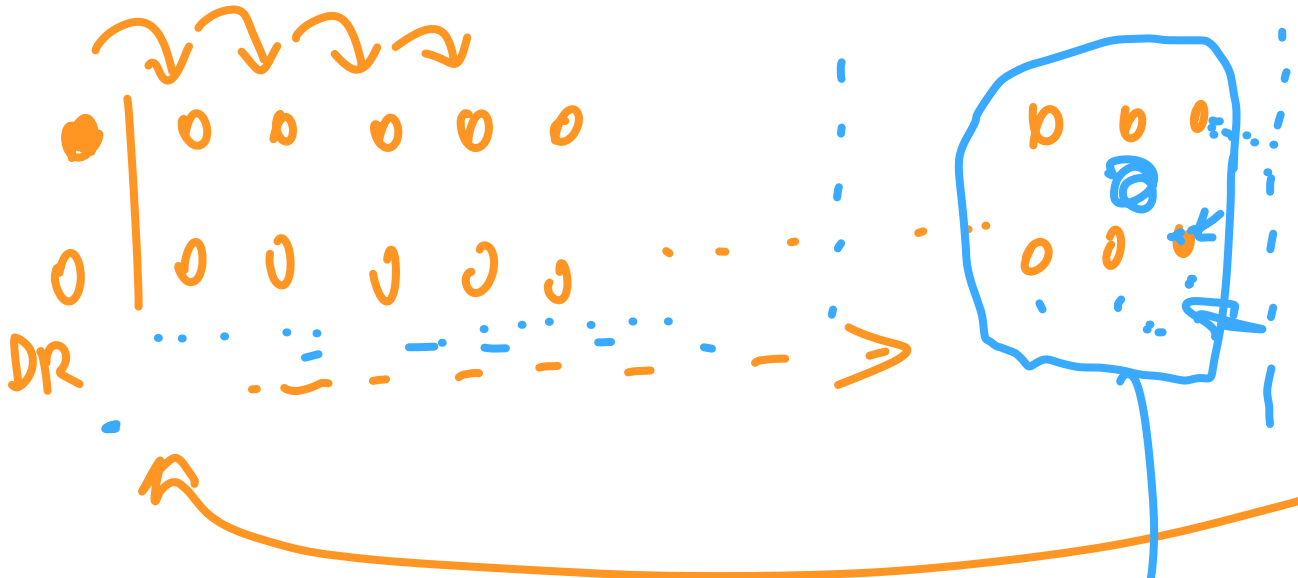
CAN BE DEMONSTRATED WITH ENERGETIC. CONS


PROXIMITY EFFECT
1
0
n1
n2
1mm
1
2
3
4
5
6
1.Mm.
BISTABILITY INCREASES
THE INFO PROP EFFECTIVENES
→ SOLVES A-TECH PROBLEM.
1
0
n1
n2
0.8mm
1
2
3
4
5
6
0.8mm

HOW MANY MOL. IN A WIRE ?
EVEN UNDER STABILITY SITUATION

↓

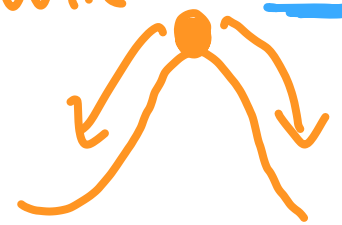
WE HAVE TO LIMIT THE NUMBER !




FIRT. ALL MOR.
RESET → NULL

↓

WHEN CK RELEASED



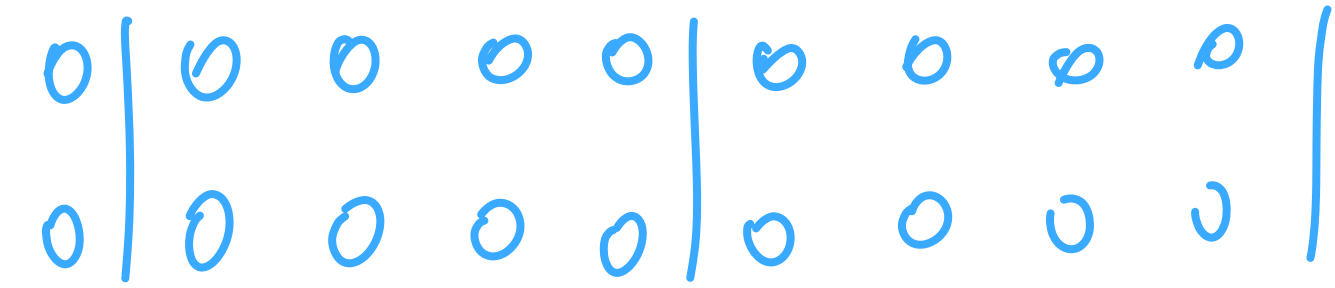
FROM THE LEFT INFO PROPAGATES
WITH A CERTAIN TIME

BEFORE ARRIVAL
OF INPUT →

MOL. AT THE END START
TO MOVE TOWARD A
STABLE STATE

→ A MAX N. OF POL EXIST IN A WIRE
TO AVOID INFO. CLASH

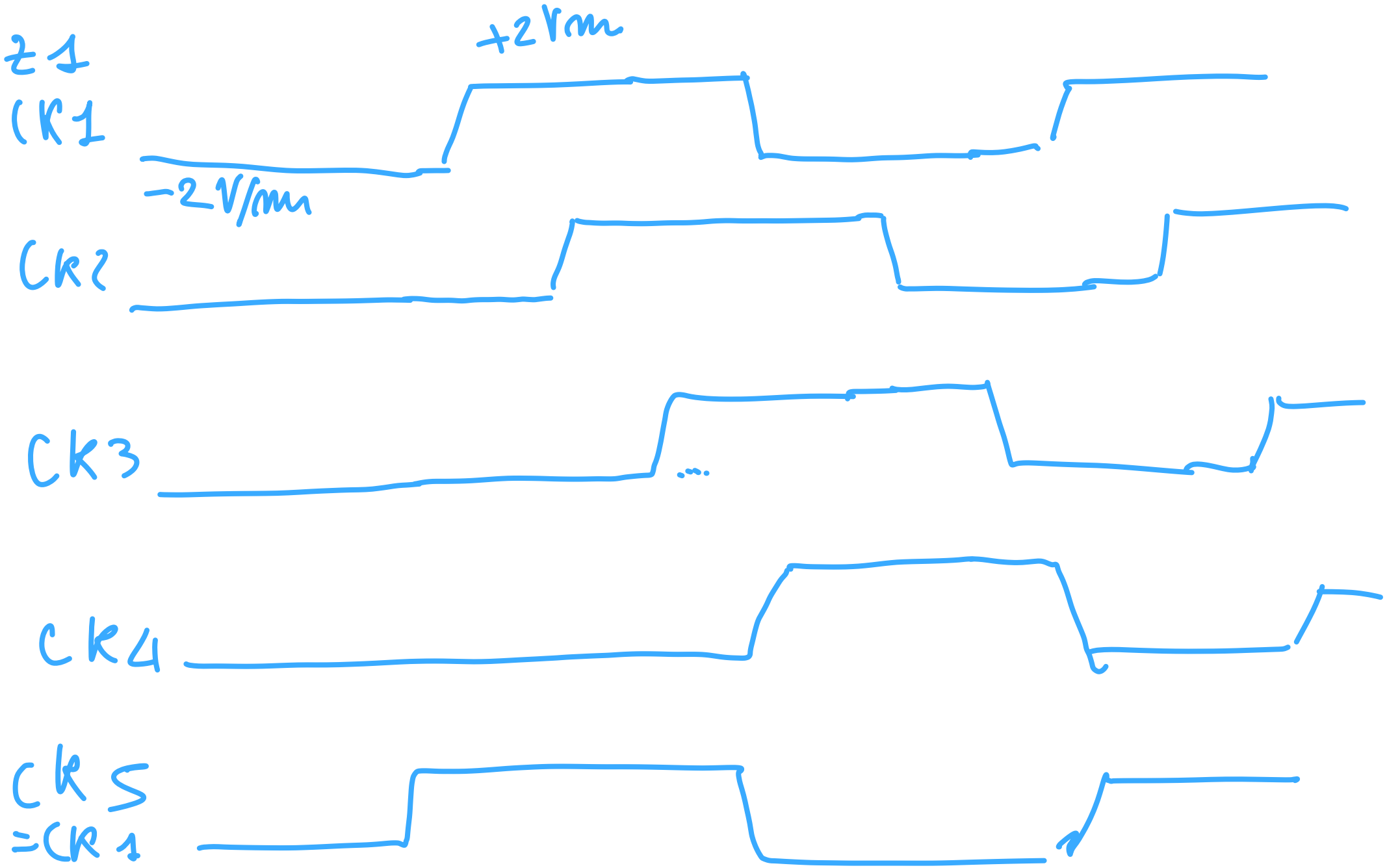
→ WE CAN USE DIFFERE CLOCK ZONES



OR

ZONE1 ZONE2 .....

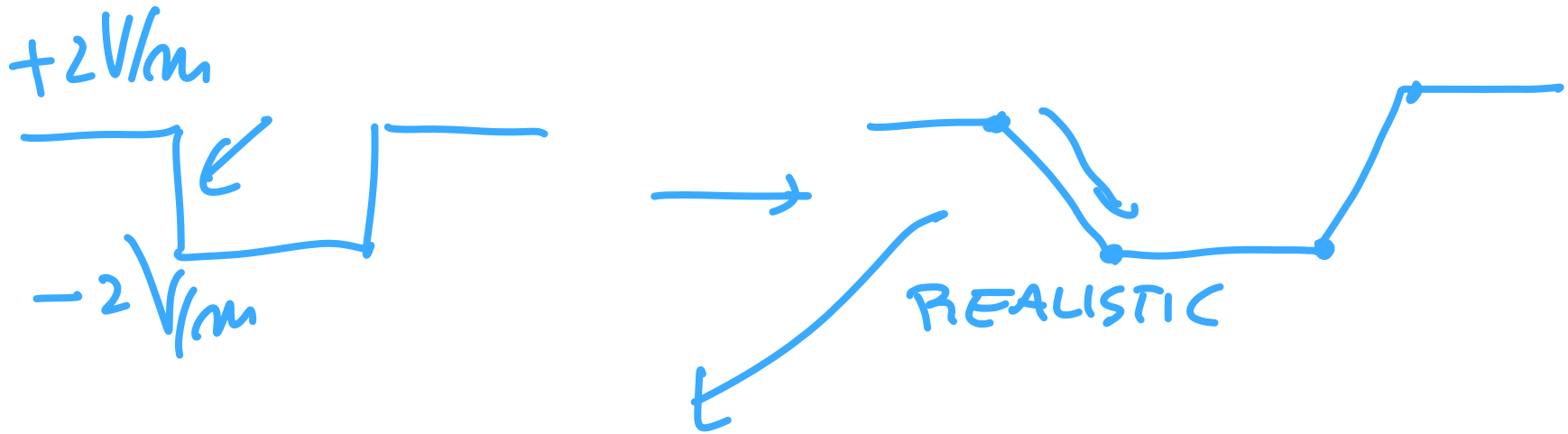
WITH DIFFERNT ZONES THE WIRE
CAN BE VERY LONG

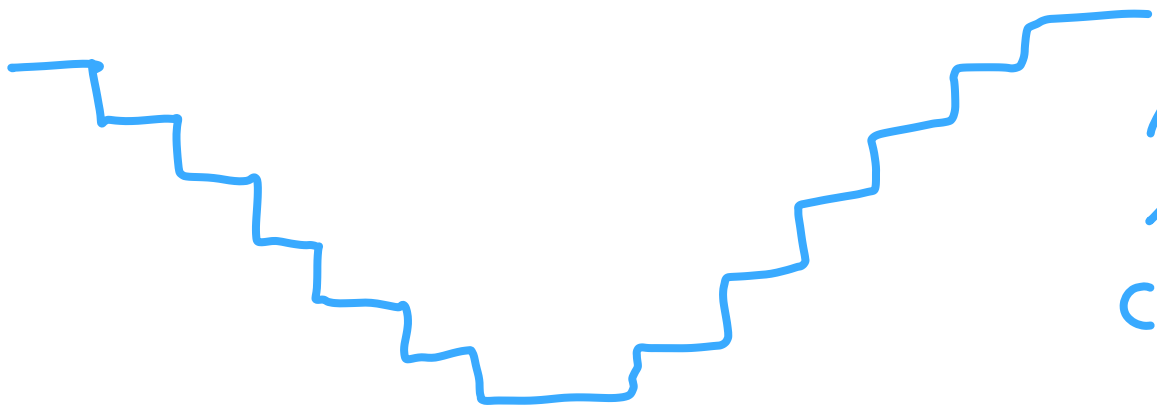

t1
+2 V/m
CK1
-2 V/m
CK2
CK3
...
CK4
CK5
=CK1

→ INCLUDE CR IN THE ALGO.

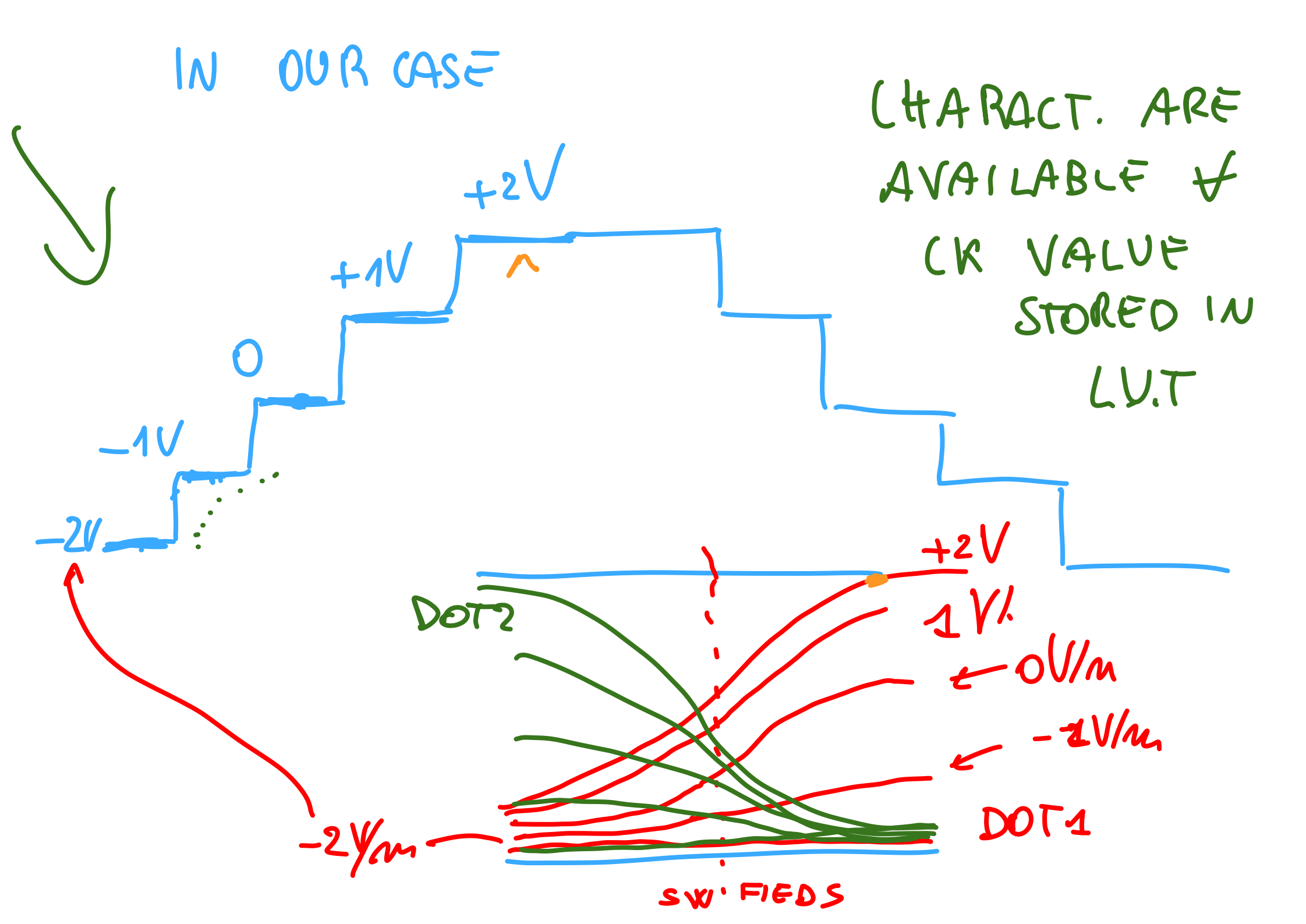
SAME PROCEDURE

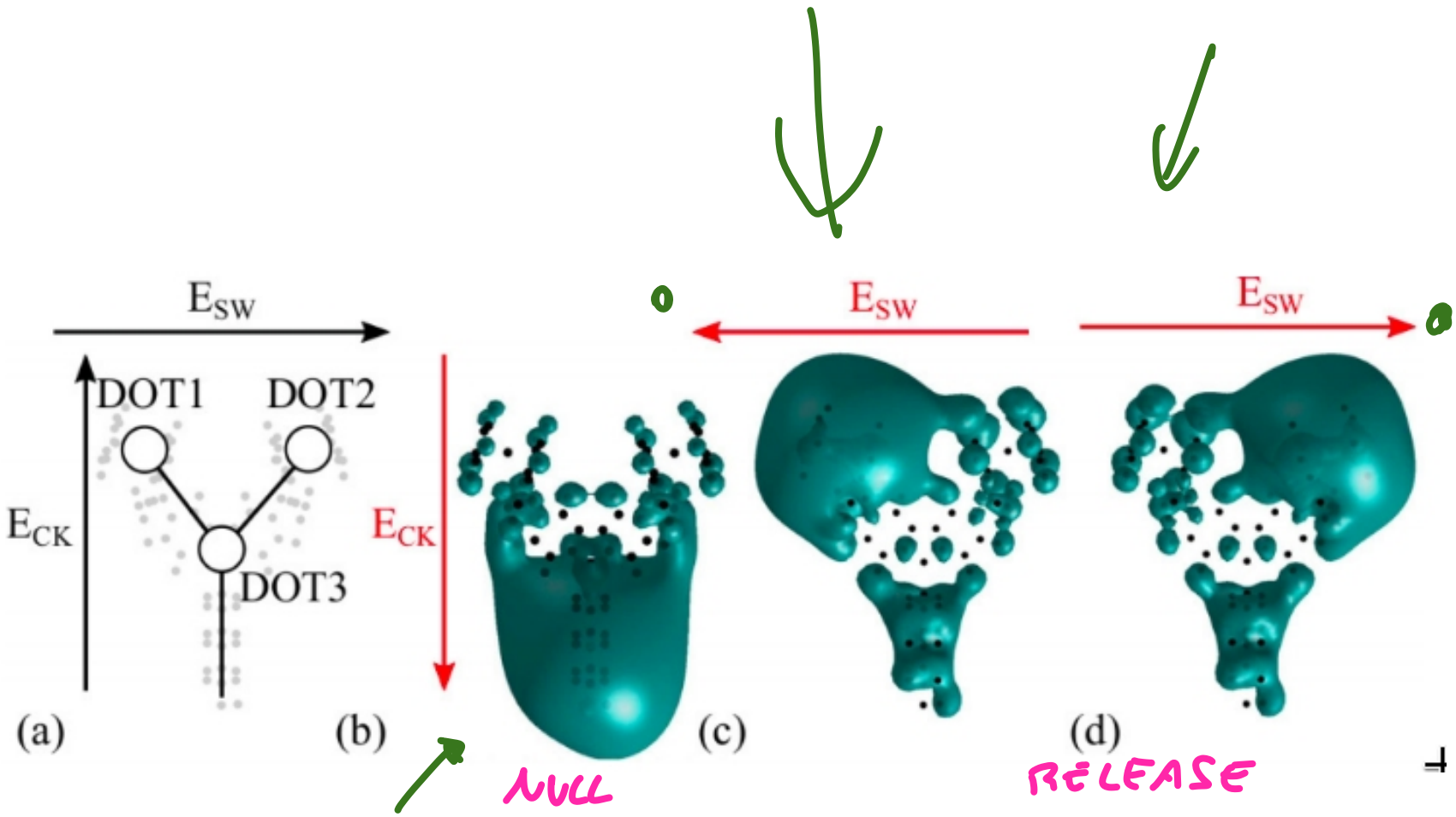
$$Q_{1i}, Q_{2i}, Q_{3i} = f(V_{inj}, CK)$$



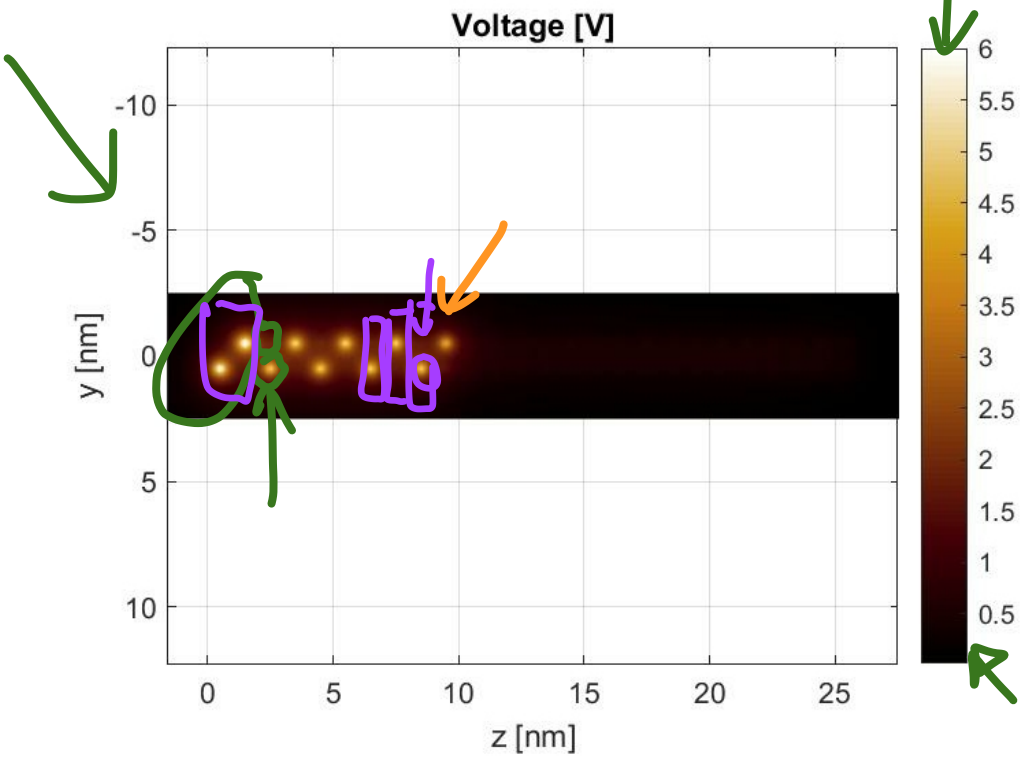
APPROX WITH A STEPWISE CHAR.

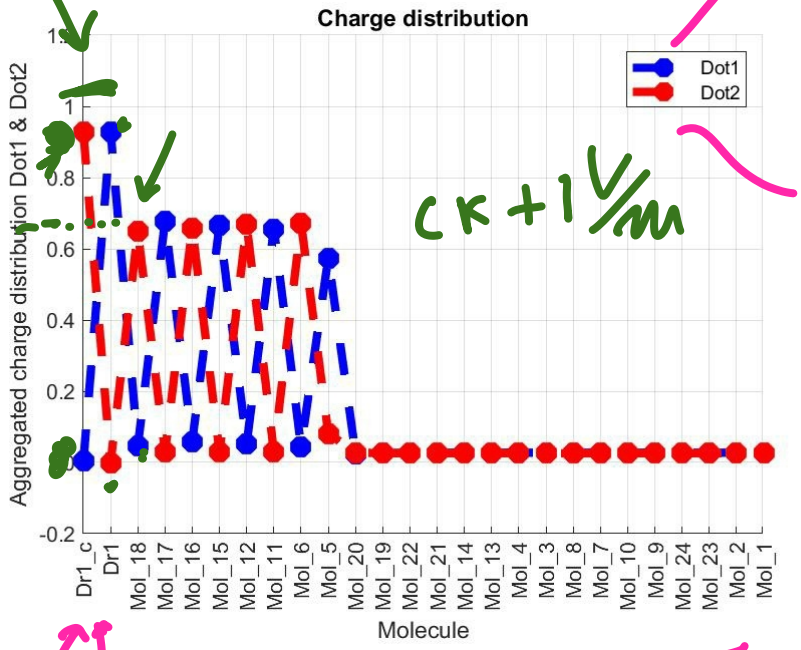

IN OUR CASE
CHARACT. ARE AVAILABLE @ CK VALUE STORED IN LUT
+2V
+1V
0
-1V
-2V
DOT2
+2V
1 V/m
0V/m
-1V/m
DOT1
-2V/m
SW FIELDS




EQUIPOTENTIAL SURFACE CALUCATED WITH DFT CALCULATION.

# 1 DRIVER + WIRE WITH 20 MOL




DOT 1

DOT 2

CK + 1 V/m

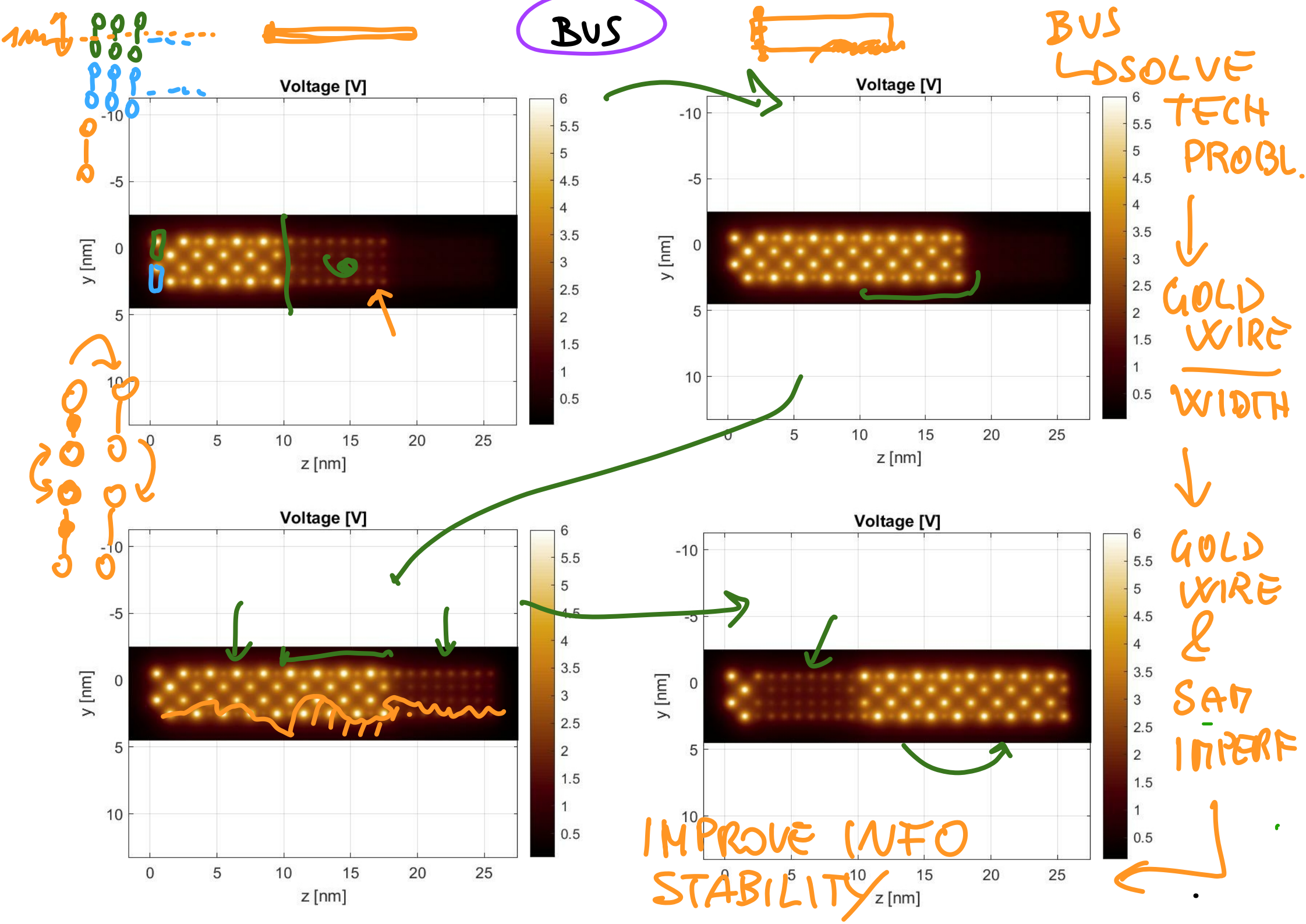
D1 D2

MOL. W WIRE

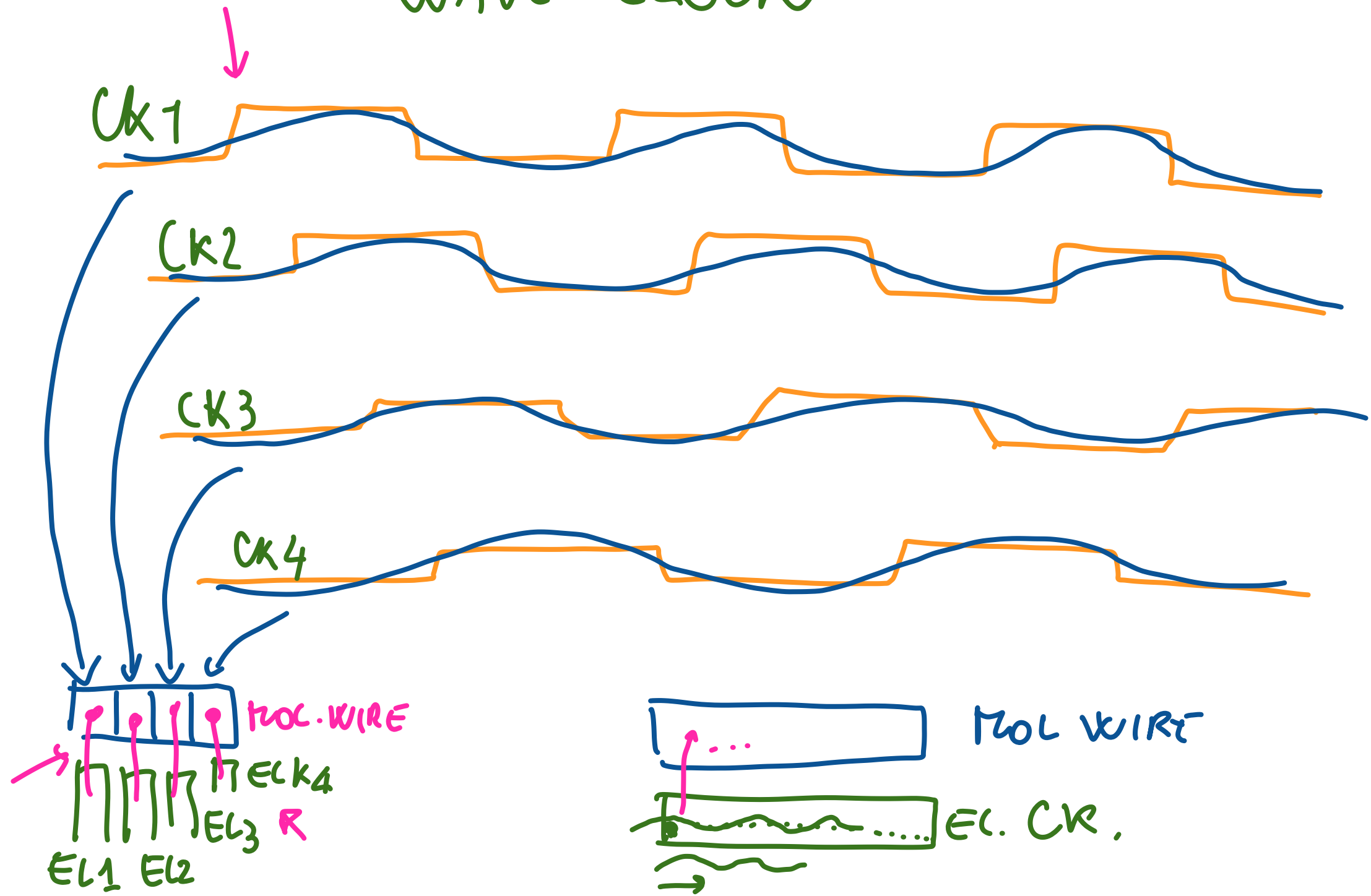
20 MOL

→ ELECTROSTATIC POTENTIAL IN THE WIRE GENERATED BY MOL. CHARGE DISTRIBUTION EVALUATED JUST ABOVE THE WIRE PLANE

SEE VIDEO


BUS
Voltage [V]
y [nm]
z [nm]
BUS
LDSOLVE
TECH
PROBL.
GOLD
WIRE
WIDTH
GOLD
WIRE
&
SAM
IMPROVE INFO
STABILITY

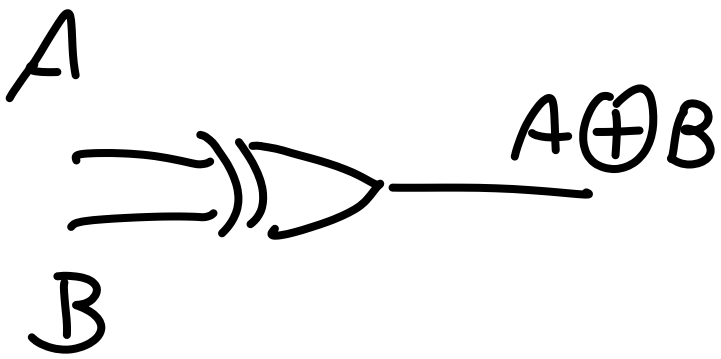
# WAVE CLOCK

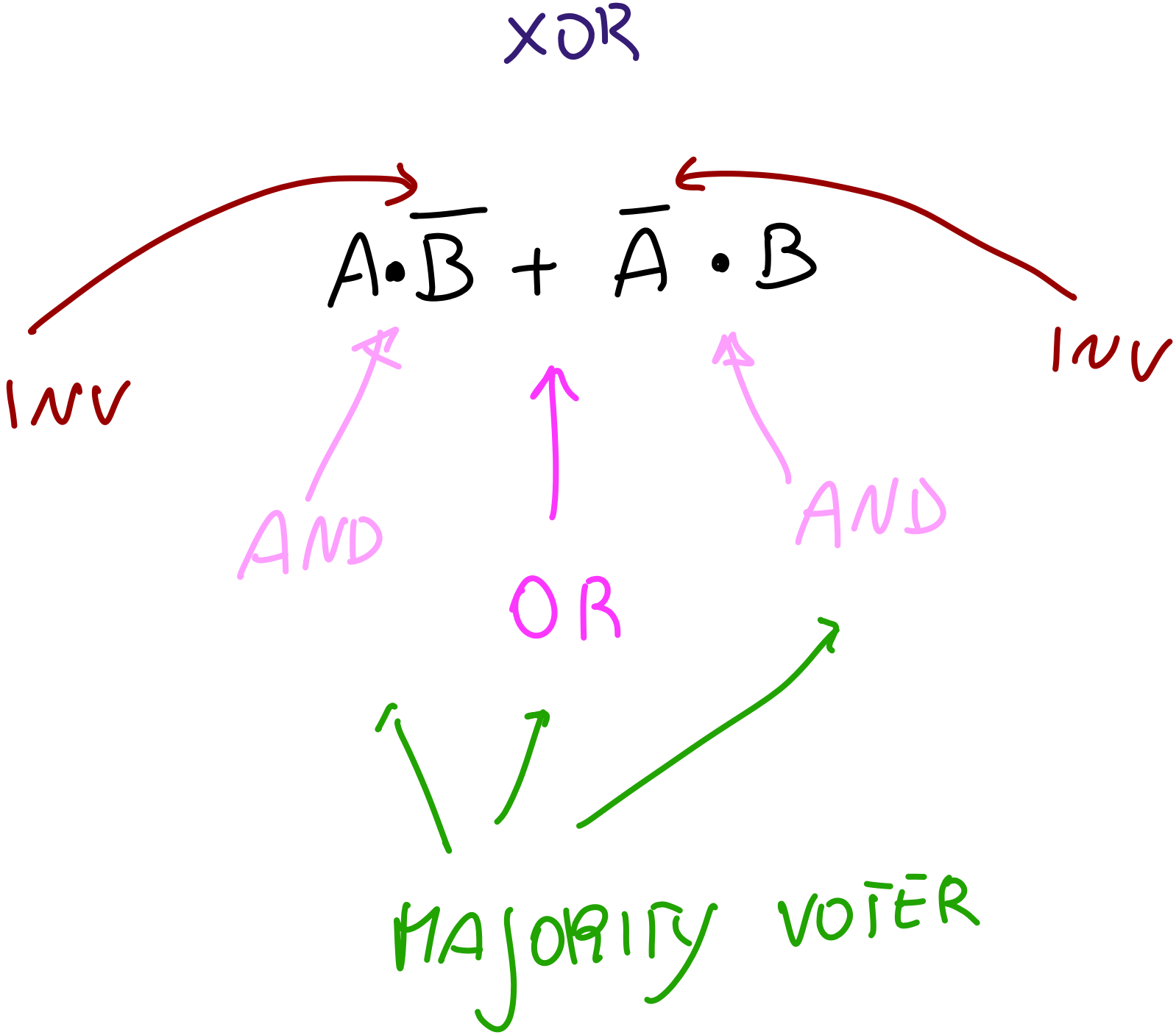


# EXERCISE

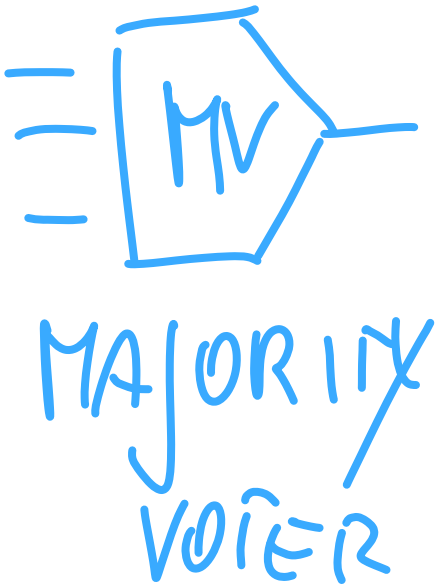
## EXAMPLE OF A GATE

XOR

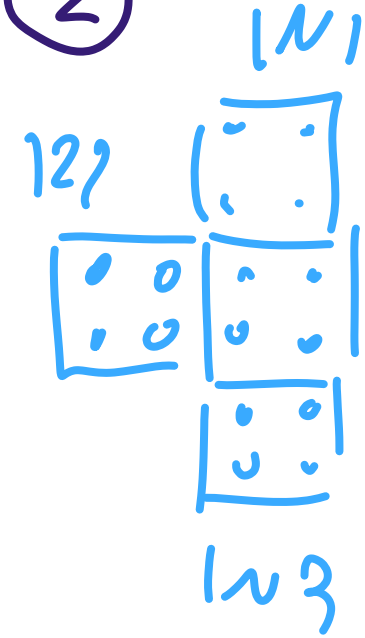



XOR
$A \cdot \overline{B} + \overline{A} \cdot B$
INV
INV
AND
OR
AND
MAJORITY VOTER

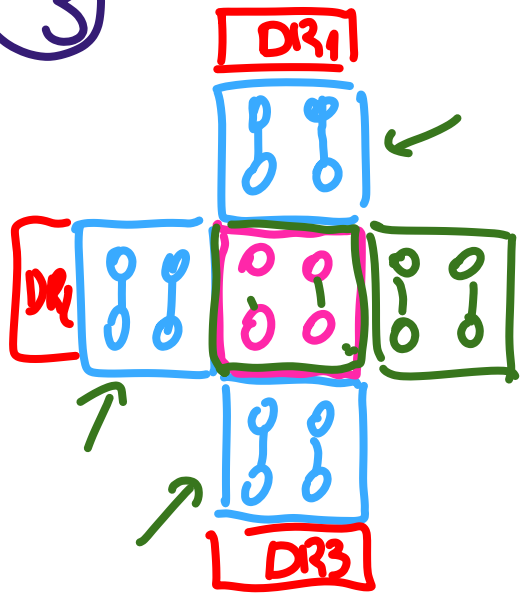
1


MV
MAJORITY
VOTER

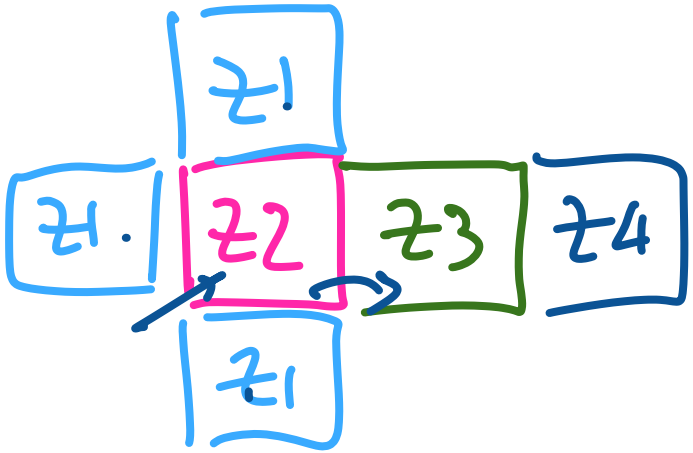
2


IN1
IN2
IN3

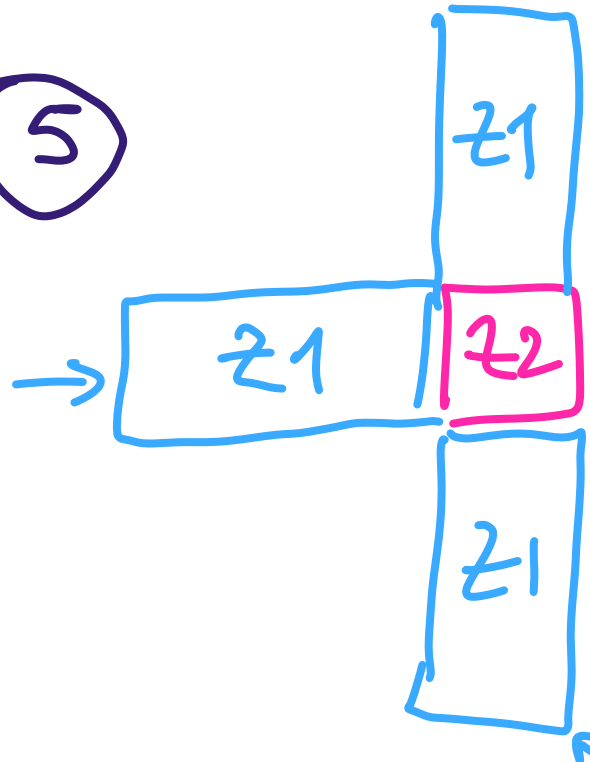
3

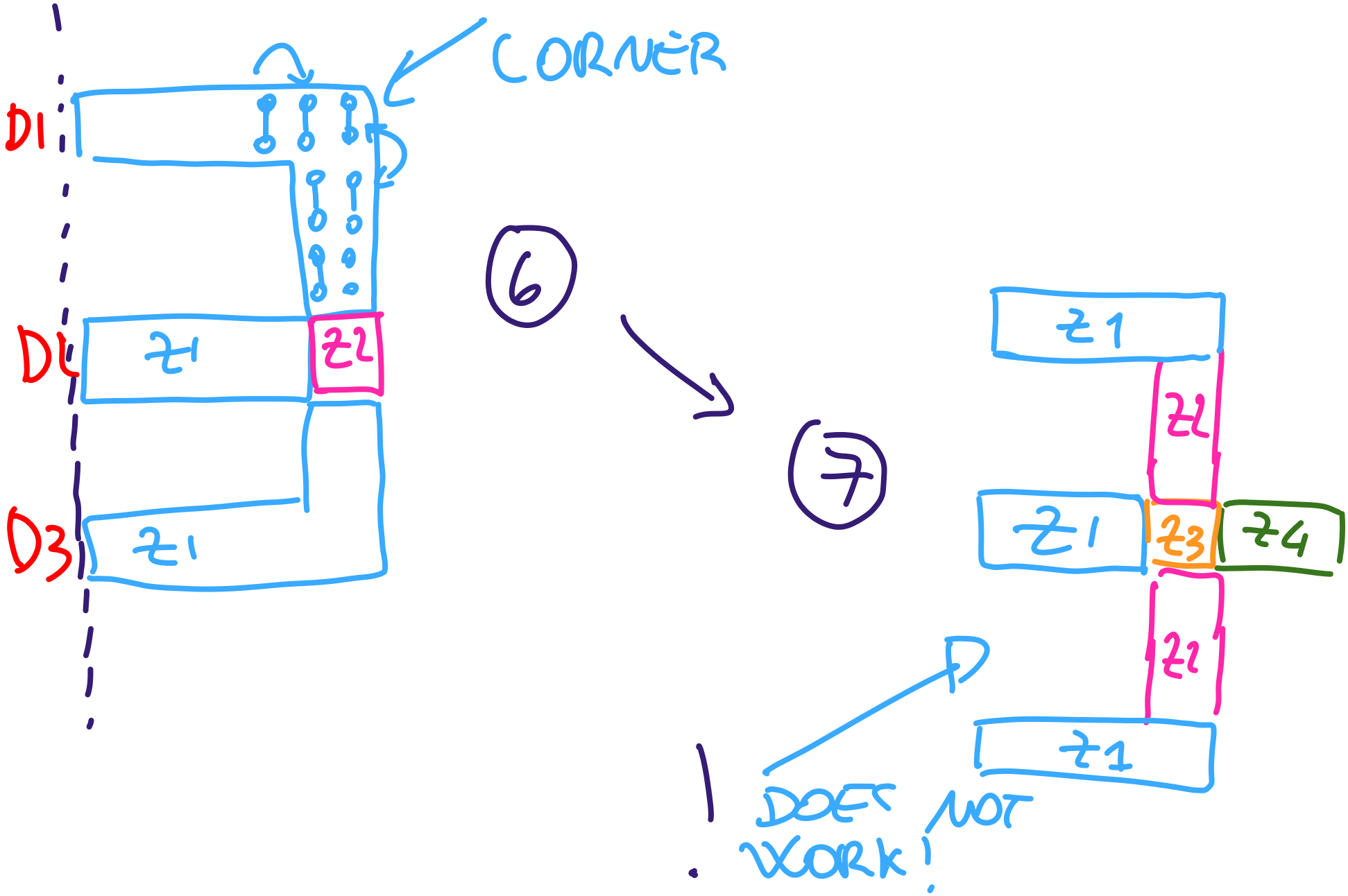

DR1
DR2
DR3

4

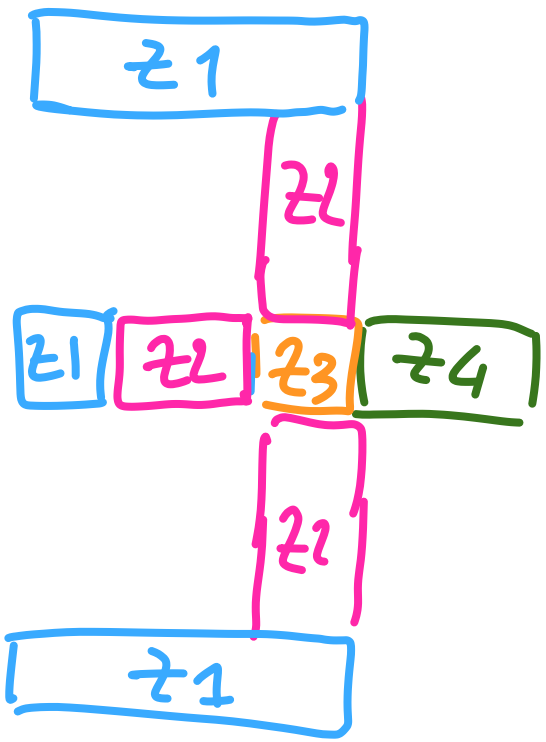

Z1
Z1
Z2
Z3
Z4
Z1

5


Z1
Z1
Z2
Z1


CORNER
D1
D2
D3
Z1
Z2
Z1
Z1
6
7
Z1
Z2
Z1
Z3
Z4
Z1
Z1
DOES NOT WORK!

8



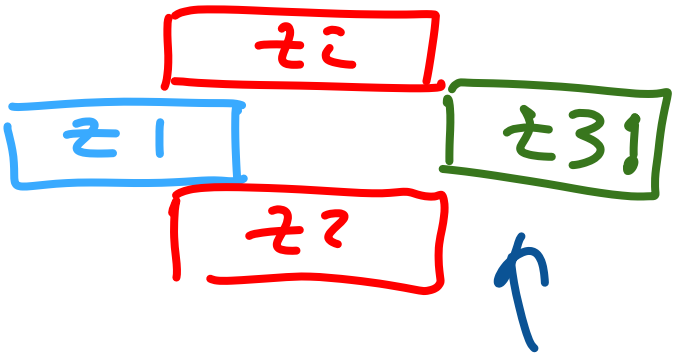

THE SAME N. OF UR. ZONES FROM INPUT

SKEWING!

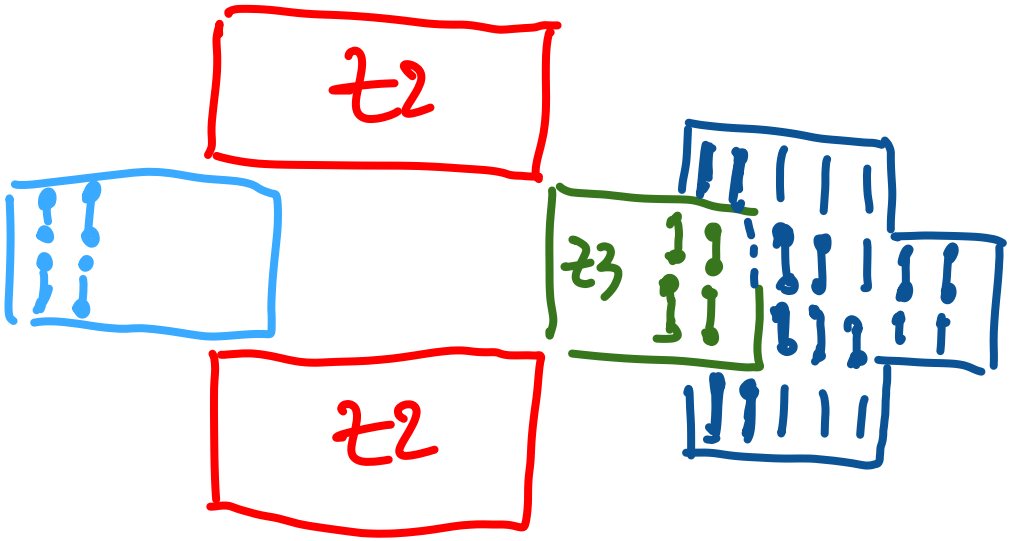
LAYOUT = TIMING

INVERTER

9




↓ HERE THE BUS HECPS!

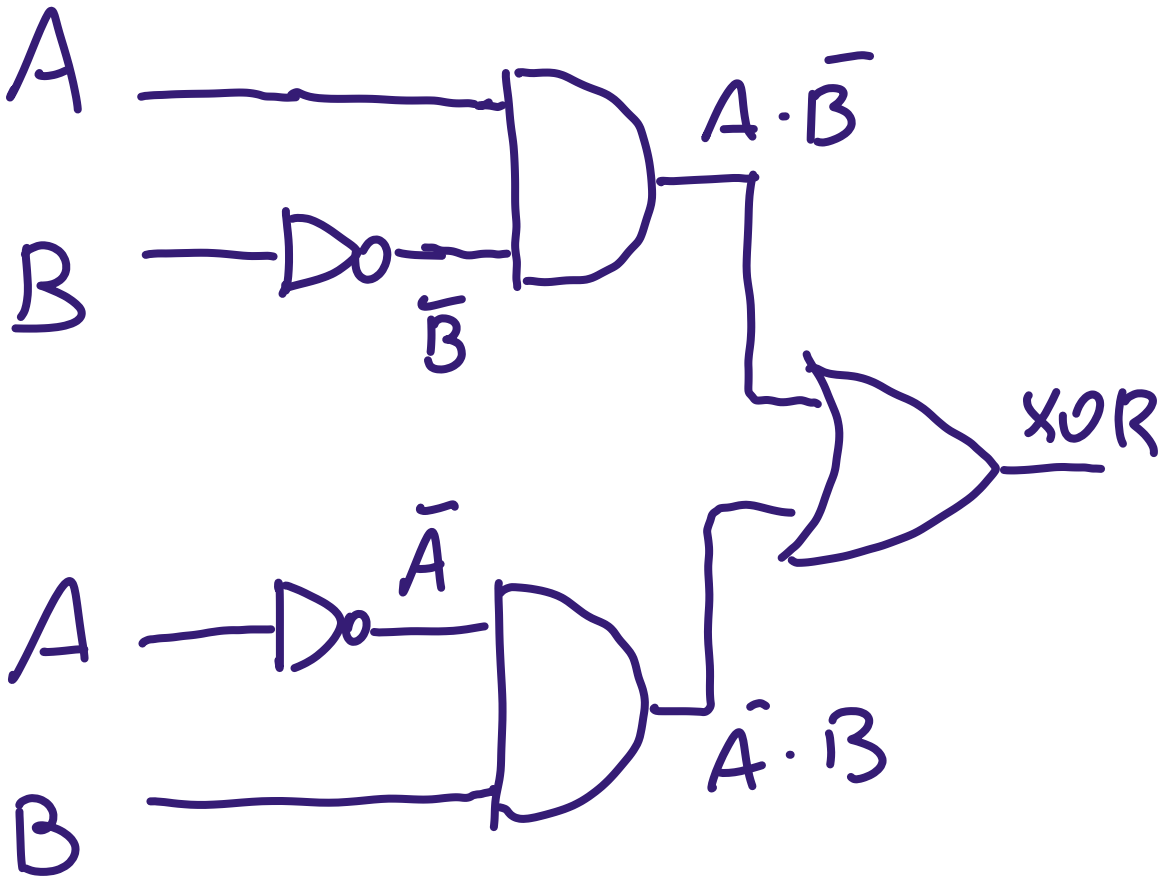


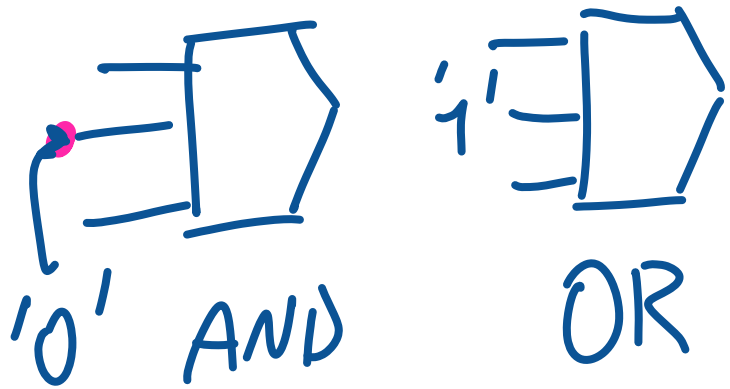

10

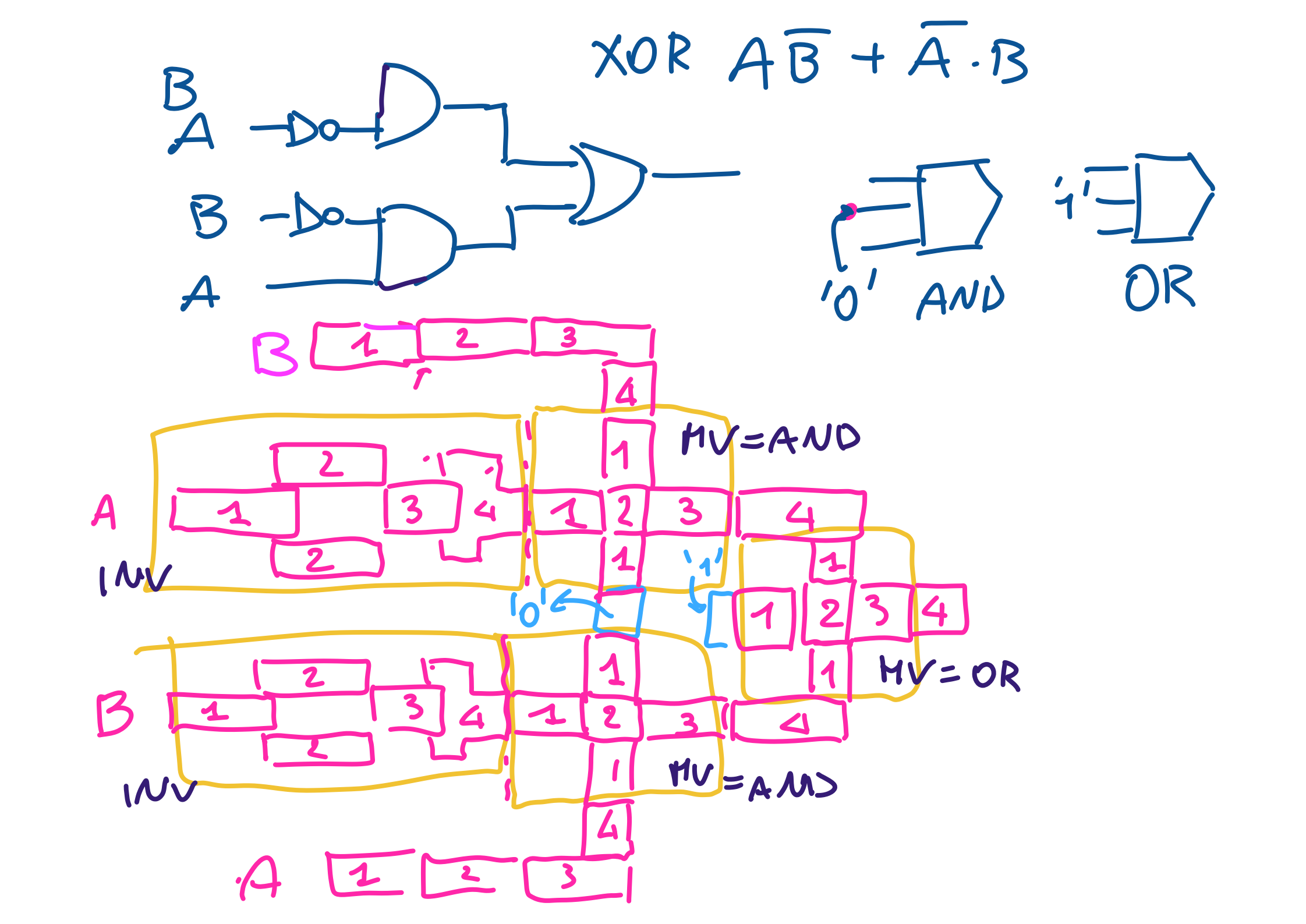
SAFER

# XOR

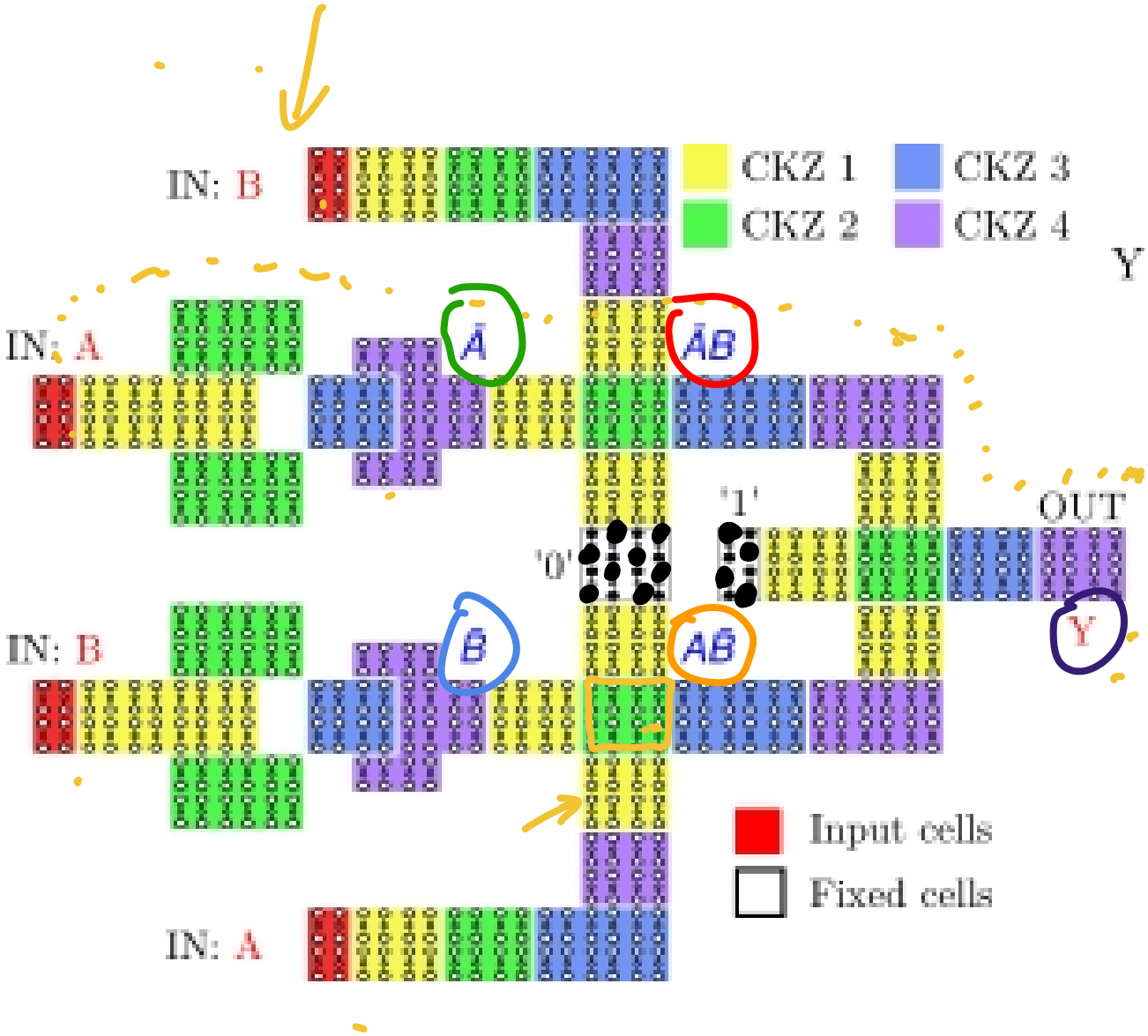
$A \cdot \bar{B} + \bar{A} \cdot B$




XOR $A\overline{B} + \overline{A} \cdot B$
B
A
B
A
'0'
AND
'1'
OR
B
A
INV
MV=AND
'0'
'1'
B
INV
MV=OR
MV=AND
A

# XOR - BUS OF 2 NOL




$$Y = MV\left(\underbrace{MV(\bar{A},B,0)}_{\bar{A}B},1,\underbrace{MV(A,\bar{B},0)}_{A\bar{B}}\right)$$

| Time | A | B | $\bar{A}$ | $\bar{B}$ | $\bar{A}B$ | $A\bar{B}$ | Y |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | | | | | |
| T | 0 | 1 | 1 | 1 | | | |
| 2T | 1 | 0 | 1 | 0 | 0 | 0 | |
| 3T | 1 | 1 | 0 | 1 | 1 | 0 | 0 |
| 4T | | | 0 | 0 | 0 | 1 | 1 |
| 5T | | | | | 0 | 0 | 1 |
| 6T | | | | | | | 0 |

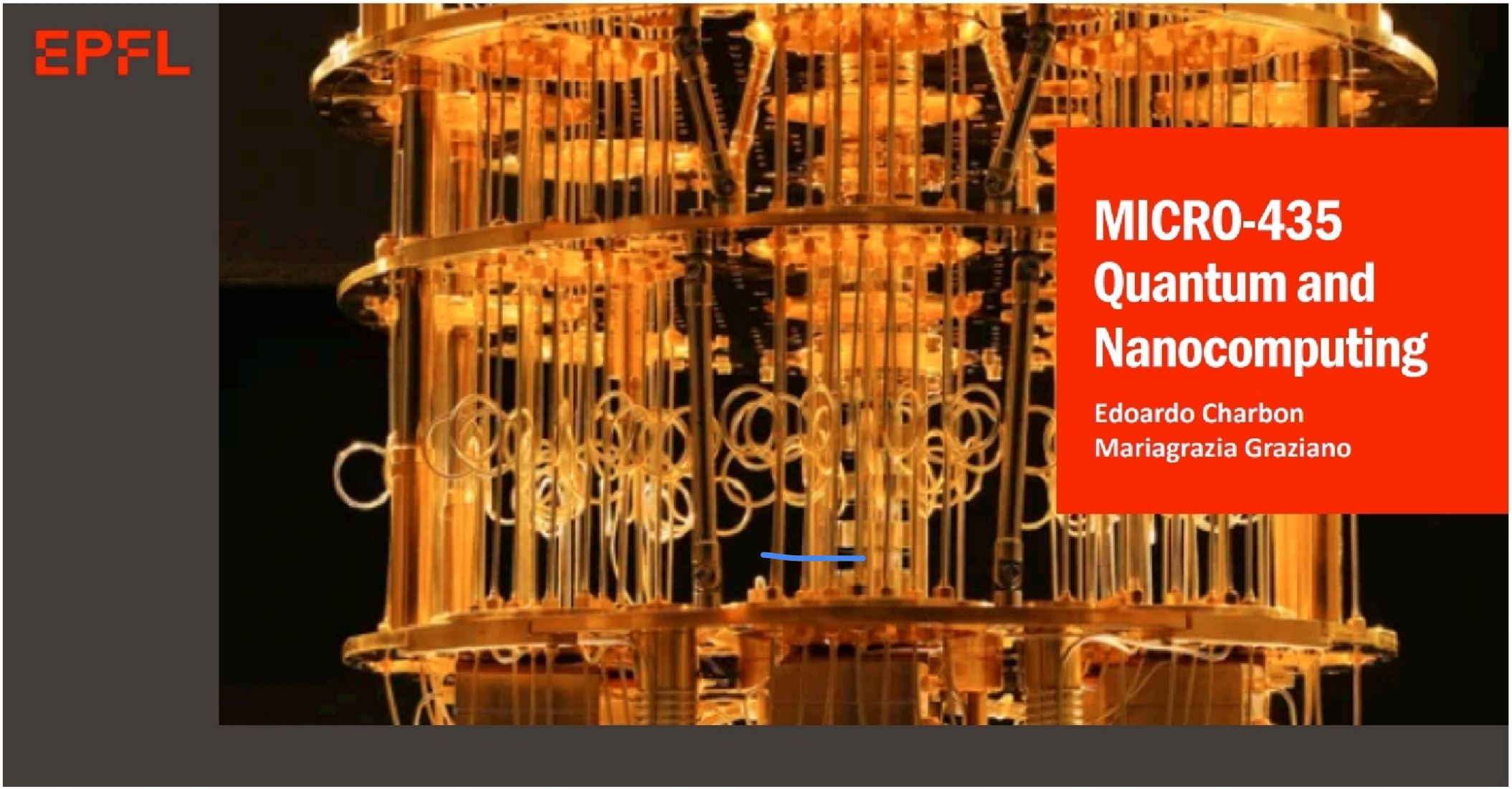
SEE VIDEO

PLA:

HA

FA

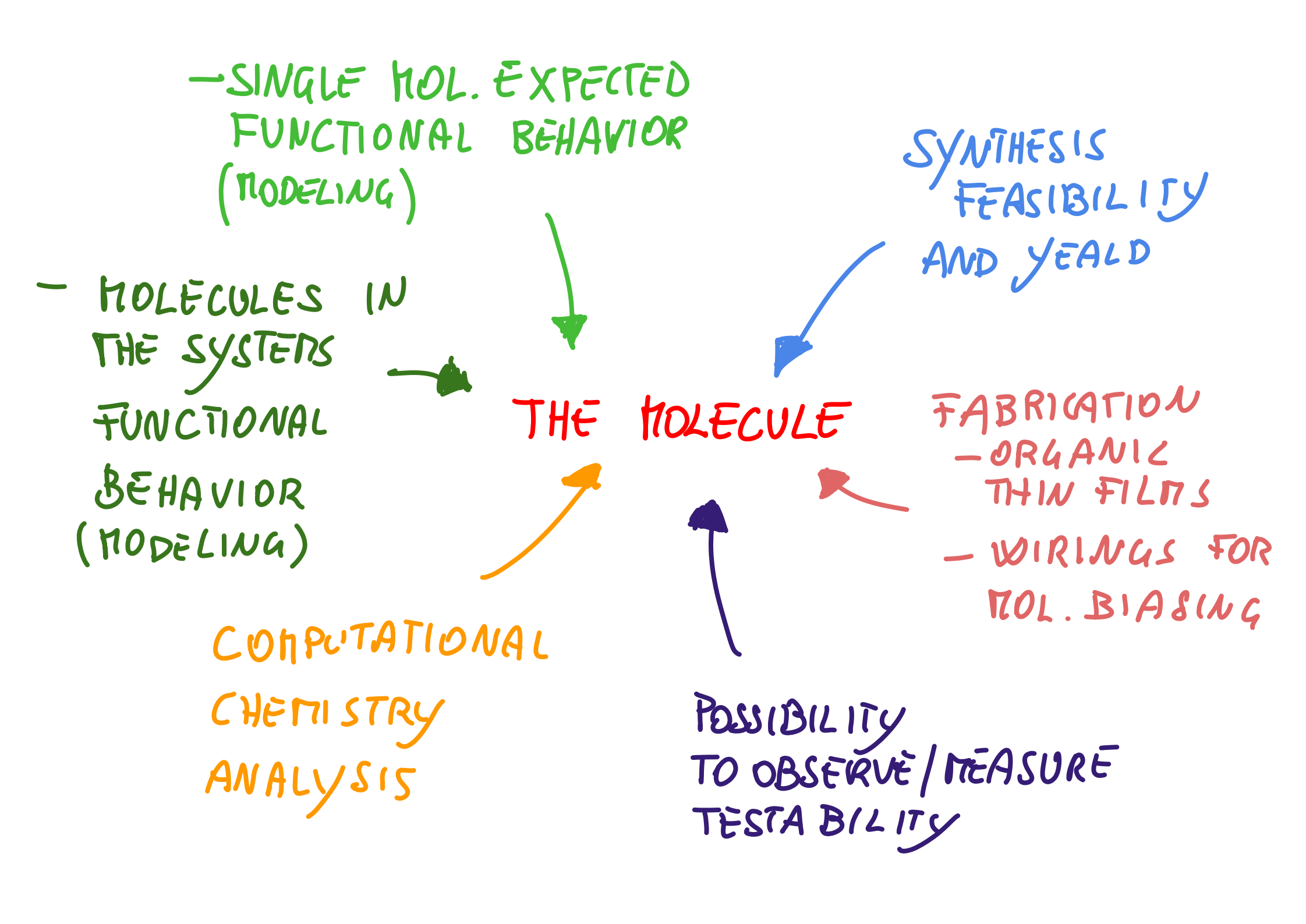
OTHER SMALL CIRCUIT



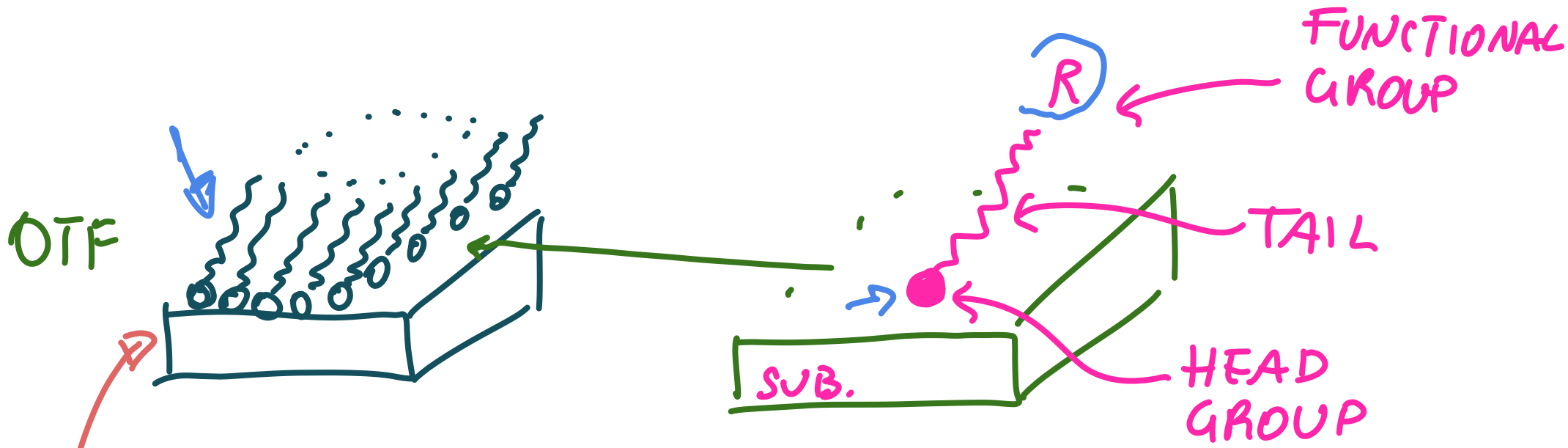

MOLECULAR FCN TECHNOLOGY

# OBJECTIVES

1) THE BASIC MOLECULE - HOW TO SELECT
2) THE FCNTOL STRUCTURE & PARAMETERS
3) MOLECULAR DYNAMICS SIMULATIONS


- SINGLE MOL. EXPECTED FUNCTIONAL BEHAVIOR (MODELING)
SYNTHESIS FEASIBILITY AND YEALD
- MOLECULES IN THE SYSTEMS FUNCTIONAL BEHAVIOR (MODELING)
THE MOLECULE
FABRICATION - ORGANIC THIN FILMS - WIRINGS FOR MOL. BIASING
COMPUTATIONAL CHEMISTRY ANALYSIS
POSSIBILITY TO OBSERVE/MEASURE TESTABILITY

# BRIEF SUMMARY ON ORGANIC THIN FILMS – OTF



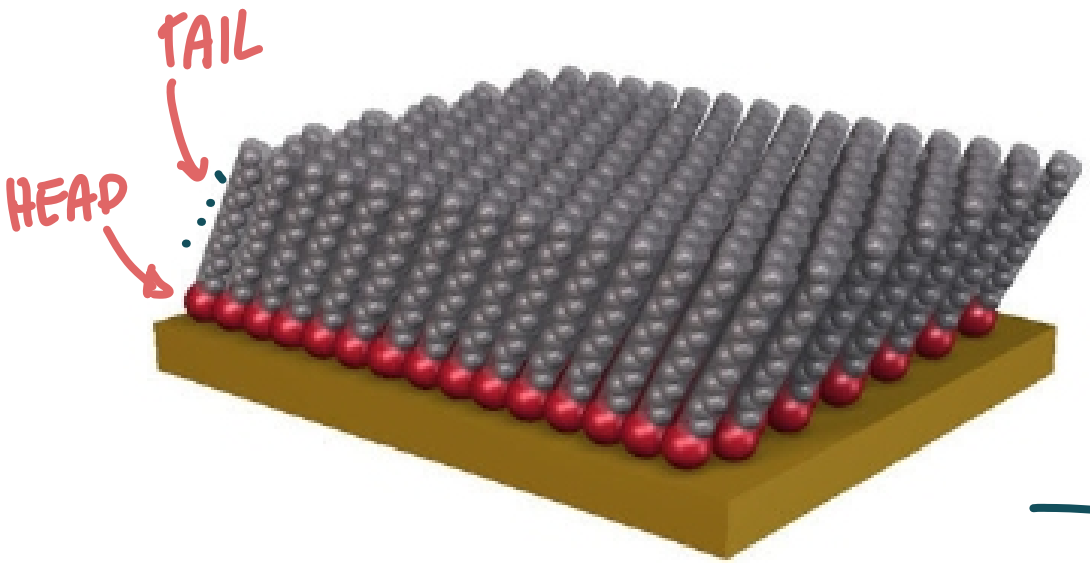

DENSE PACKED SELF ORGANIZED

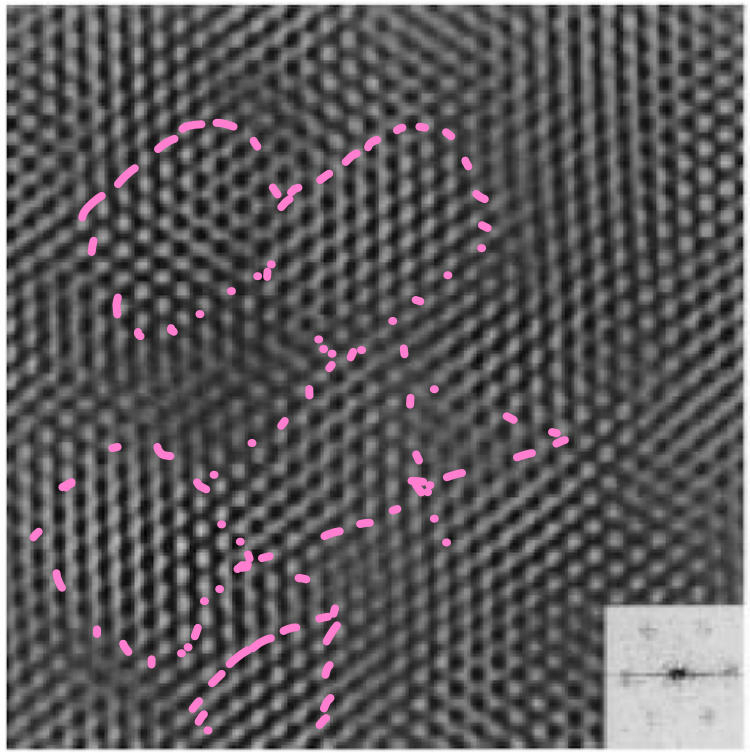
2 WAYS TO CREATE OTF

→ LANGMUIR LAYER

→ SELF-ASSEMBLY MONOLAYER - SAM

# OTF EXAMPLE



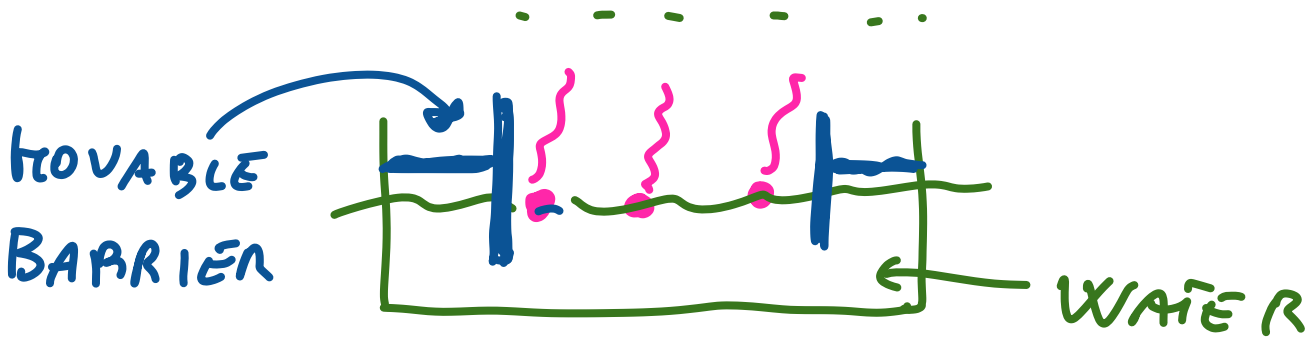



THIOL OTF - REGULAR ORIENTATION IN SUBZONES

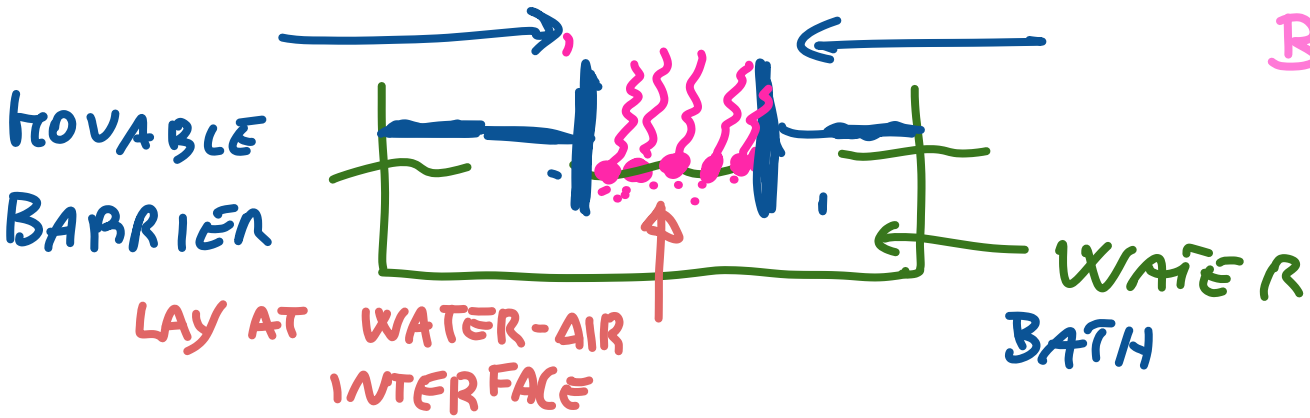
# LANGMUIR LAYER


HYDROPHOBIC REGION

HYDROPHILIC REGION



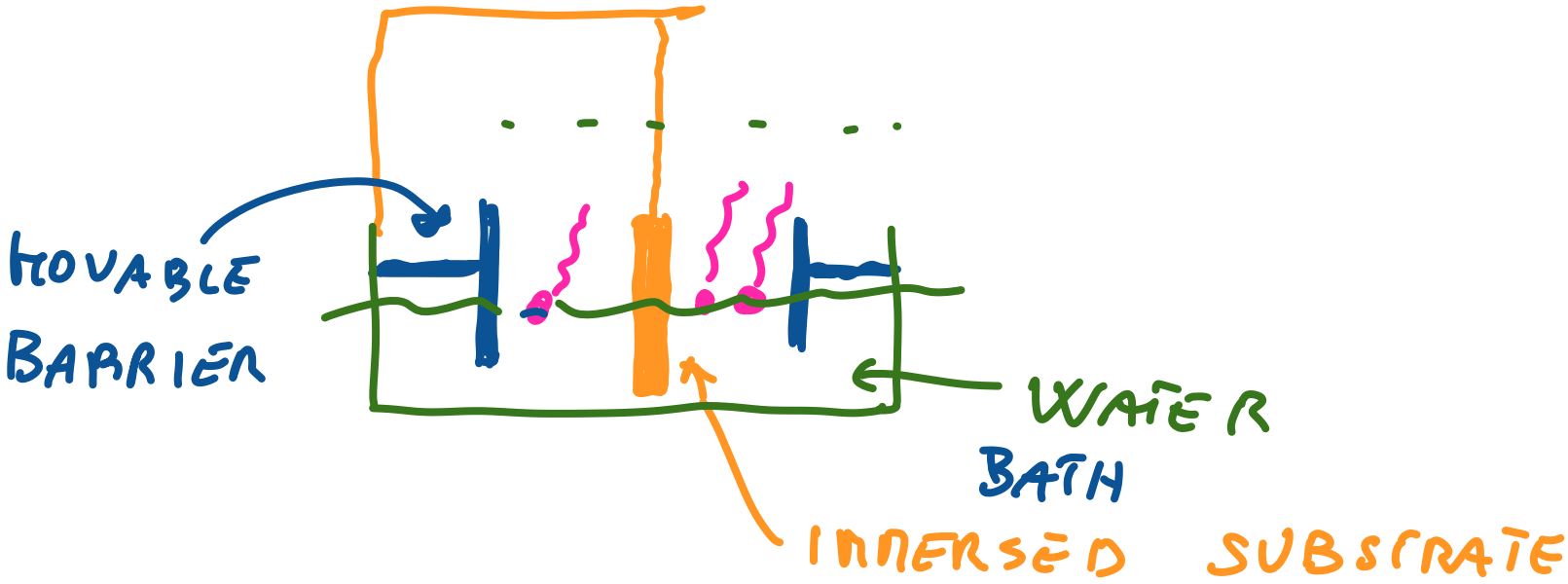

MOLECULES DEPOSITED WITH A GIVEN CONCENTRATION

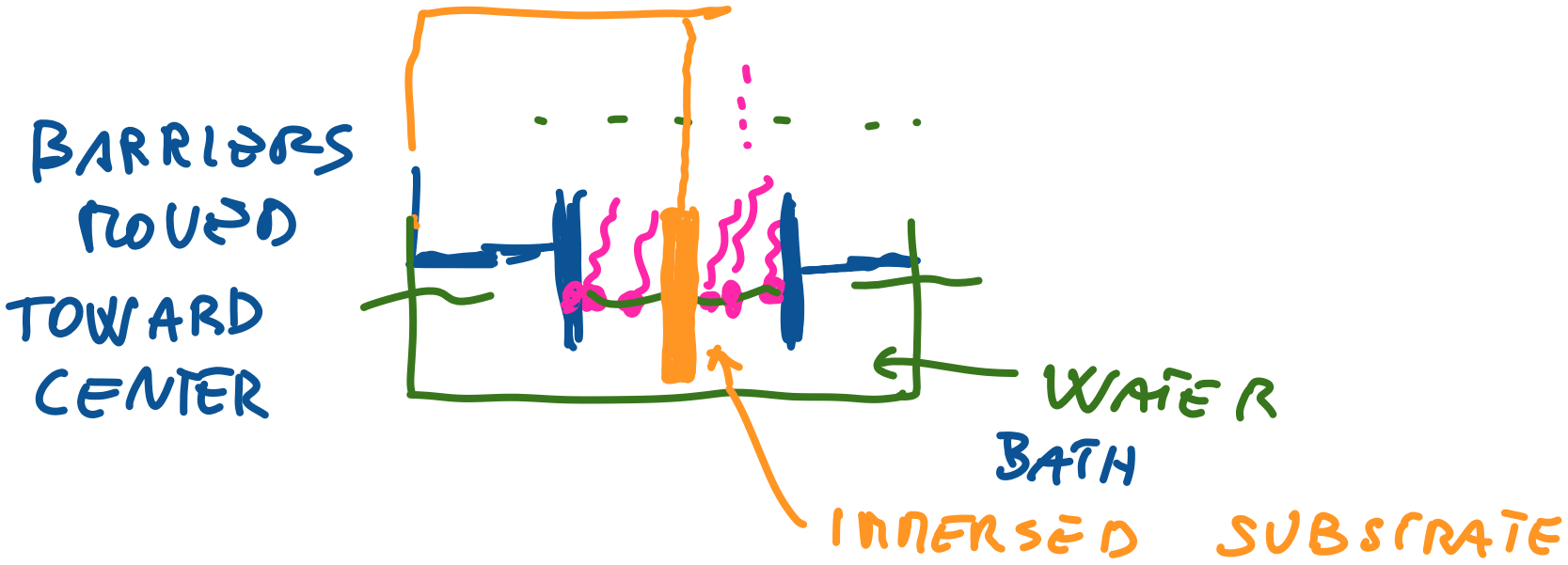



BARRIERS MOVED TOWARD THE CENTER

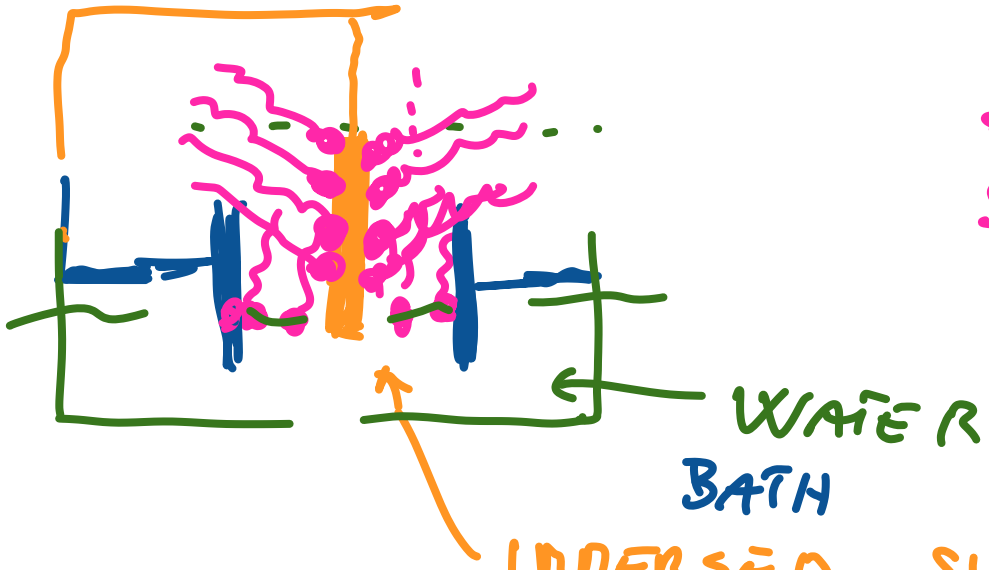
FILM CREATED

# LANGMUIR - BLODGETT (LB)



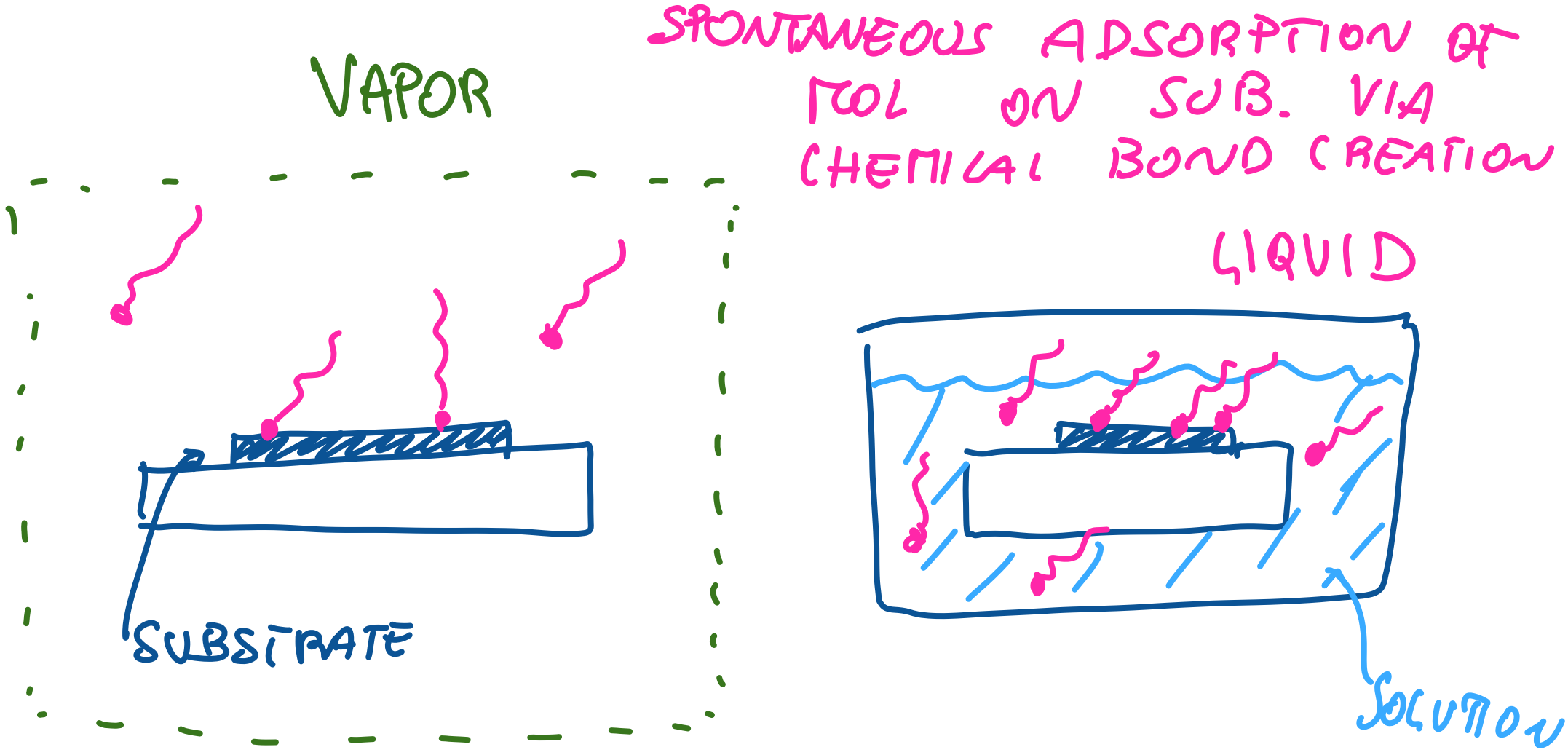
SUBSTRATE IS PULLED



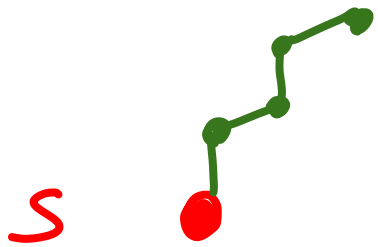

MOLECULES ATTACH IN A IN A REGULAR ORGANIZATION

THE PROCESS CAN BE ITERATED TO OBTAIN MULTICAYER LB FILMS

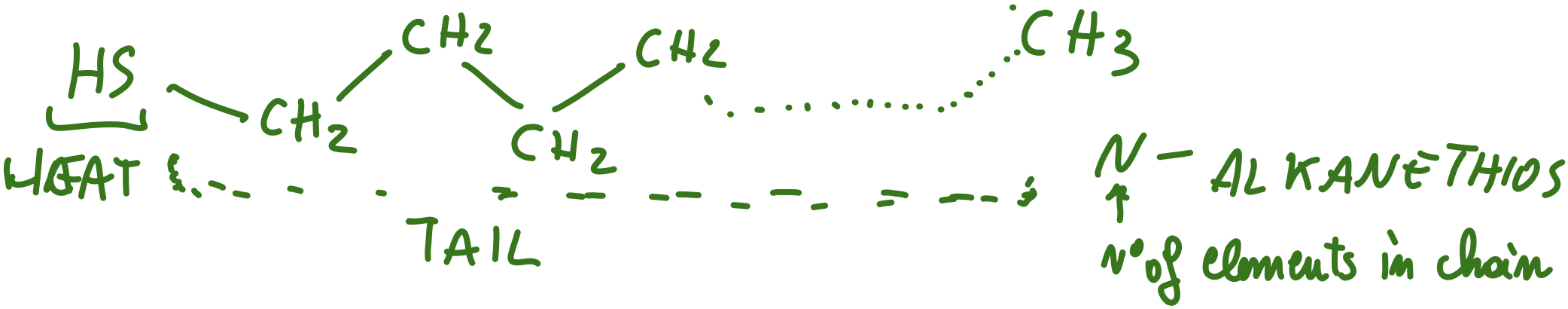
# SAM - SELF ASSEMBLED MONOLAYERS

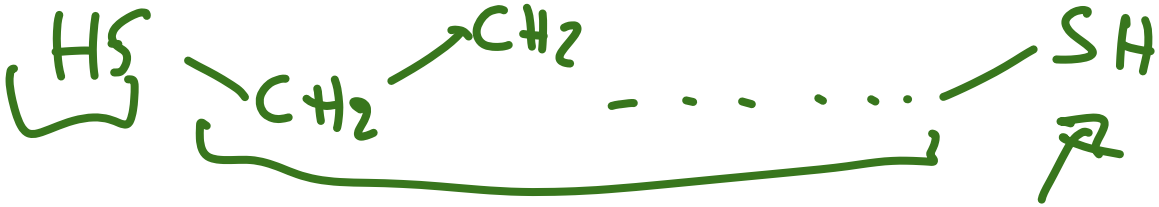


# EXAMPLE: GOLD + SULFUR




THIOL -SH

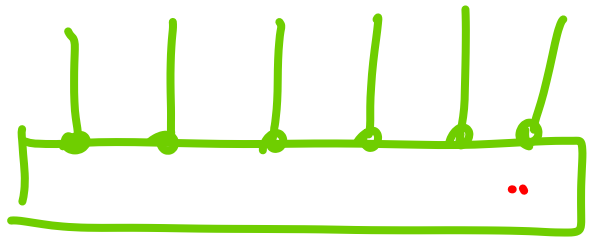




N - ALKANEDTHIOL

..... many others are possible and useful

FOR BISFERROCENE RECIPE 2 STEPS

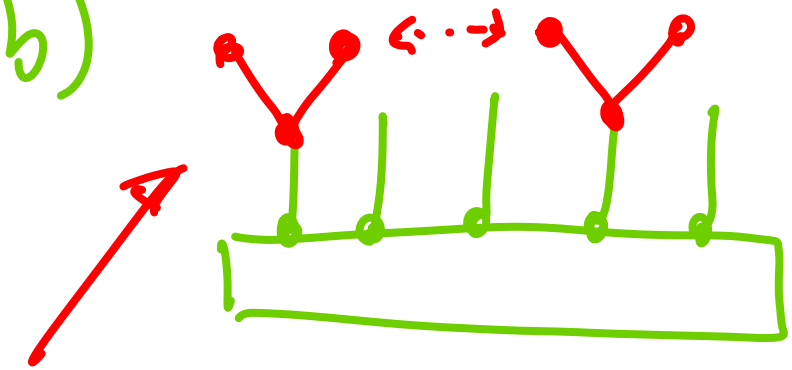
a)



SAM WITH THIOLS

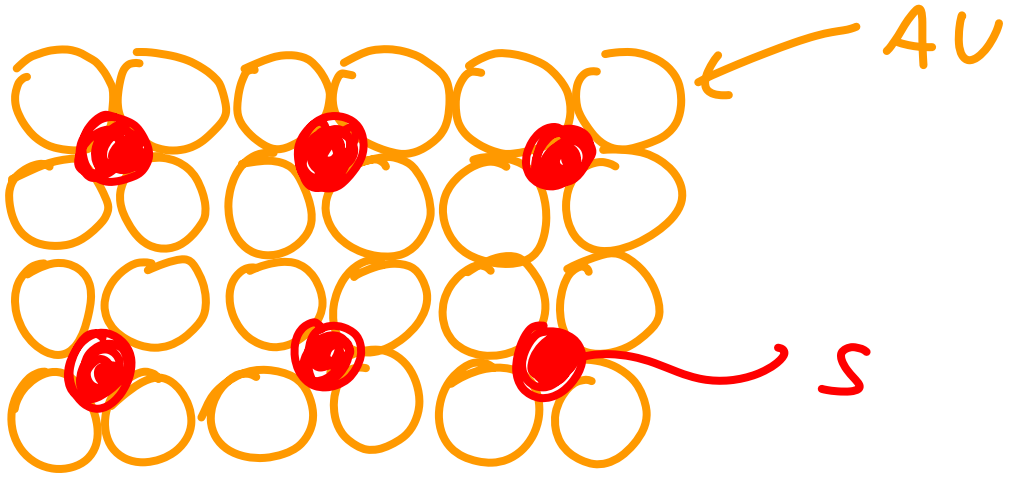
- PROPER CONCENTRATION
- // GOLD LATTICE ORIENTATION

b)



BISFERROCENE + THIOLS

HINDRANCE OF BISFERROCENES

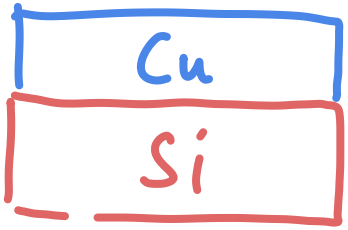



TYPICAL ATTACHMENT

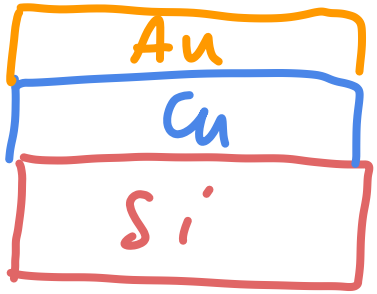
(TOP VIEW)

# SIMULATION OF THE PROCESS USING MOLECULAR DYNAMICS (LAMMPS)

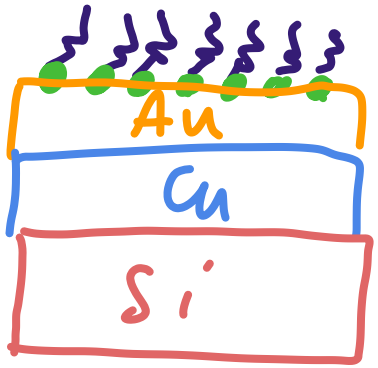

SUBSTRATE



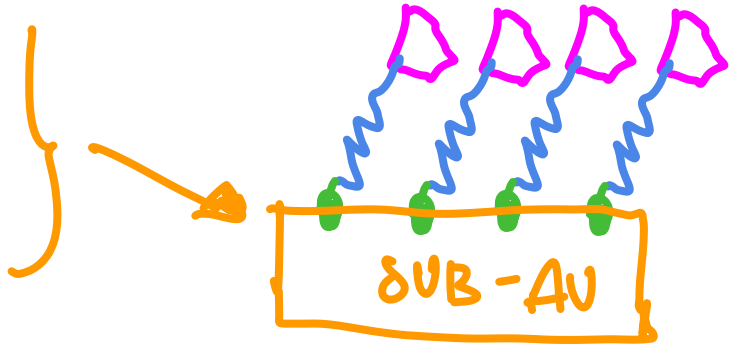

COPPER LAYER




GOLD




THIOLS

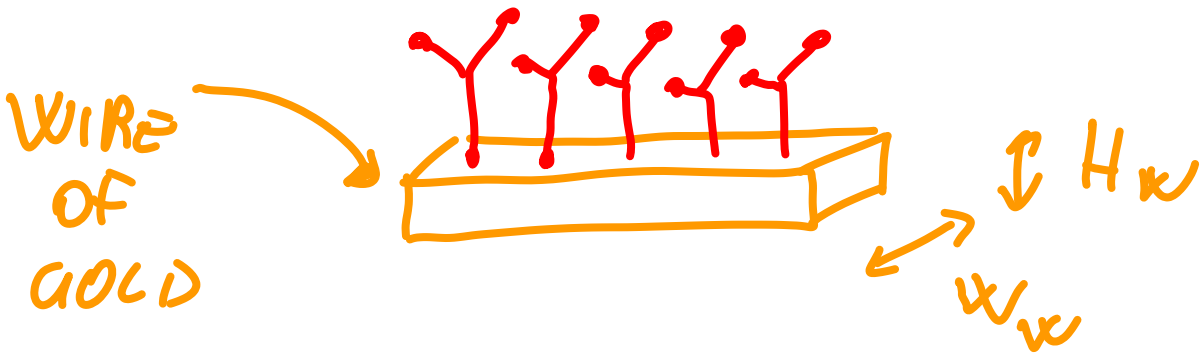


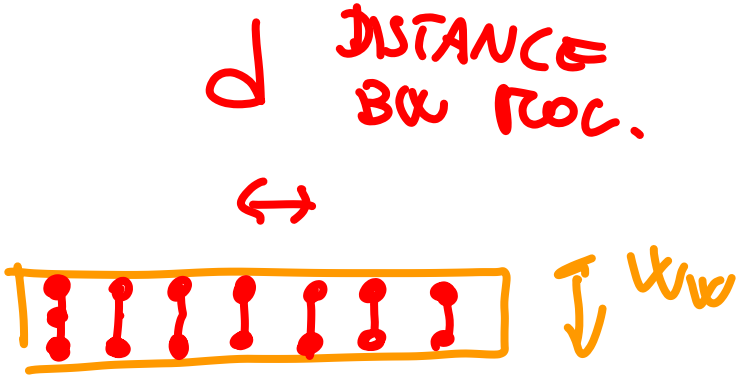

FERROCENYL - HEXANE THIOL

SINGLE FERROCENE + THIOL - COMMERCIAL THIOL.

# 2) THE MOL-FCN STRUCTURE

## 2.1) THE MOL-FCN WIRE (GUIDING WIRE)



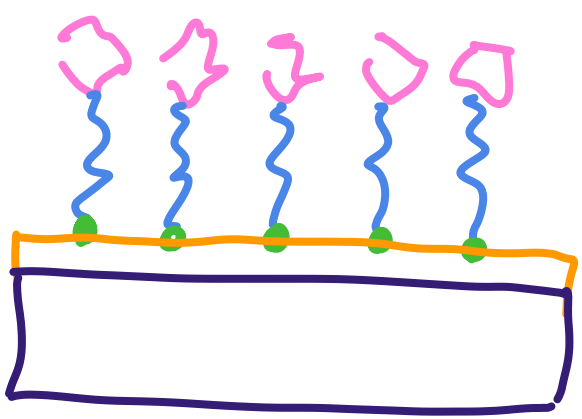



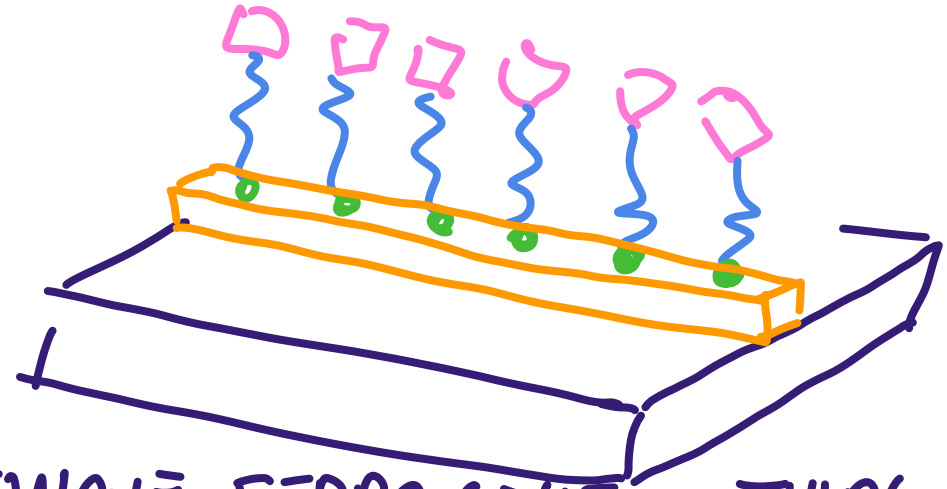

TOP VIEW

ORGANIZATION DEPENDS

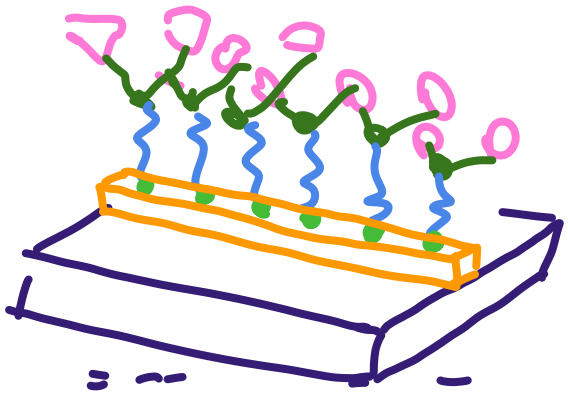
- → GOLD STR.
- → SH → ATTACHMENT
- → BISF. HINDRANCE

# MOLECULAR DYNAMICS SIMULATION



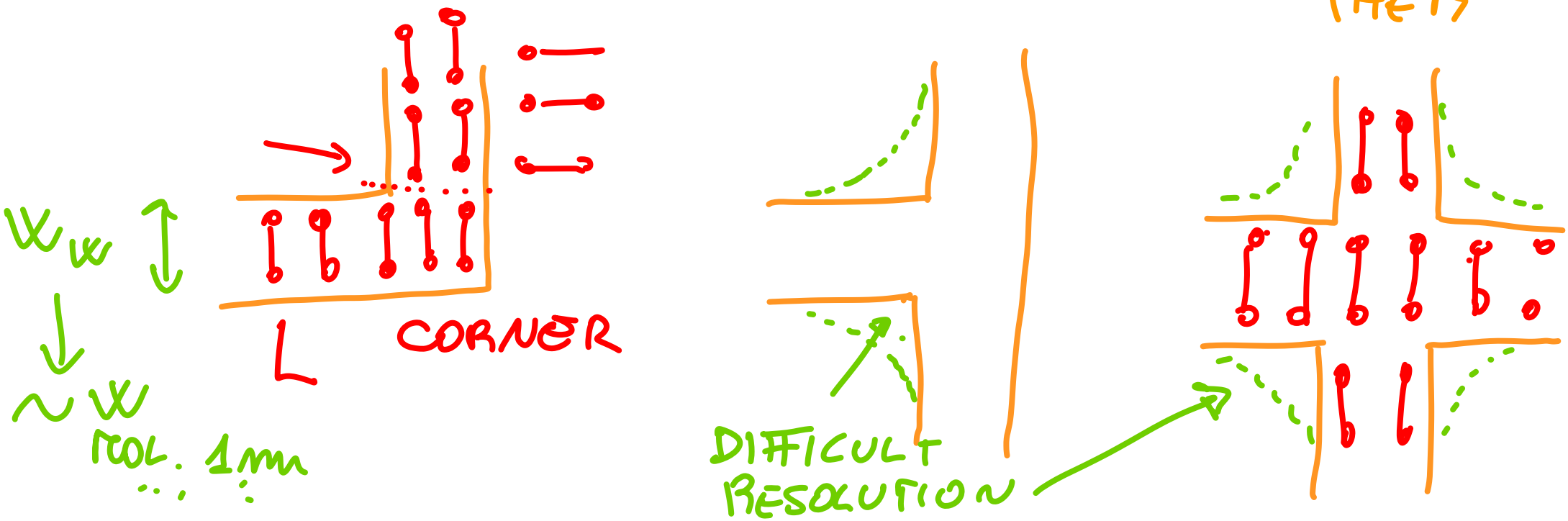


GOLD WIRE + SINGLE FERROCENE + THIOL



- OXIDIZED - NO VERTICAL CLOCK
- OXDIZED + VERTICAL CLOCK
- BISFERROCENE-THIOLATED + V. CLOCK

# 2.2.) MORE COMPLEX PATTERNS & MOLECULES DEPOSITION ON THEM

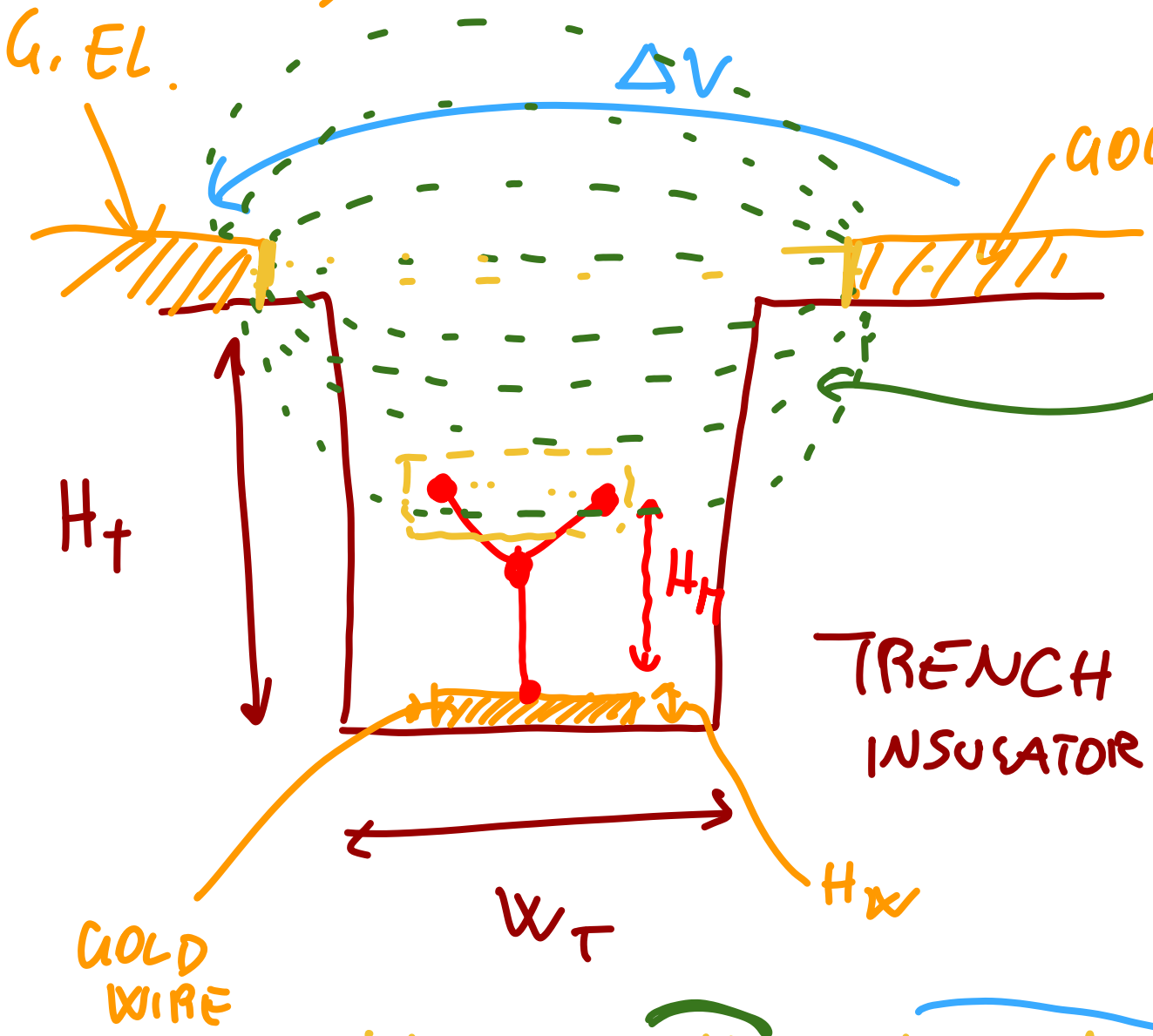


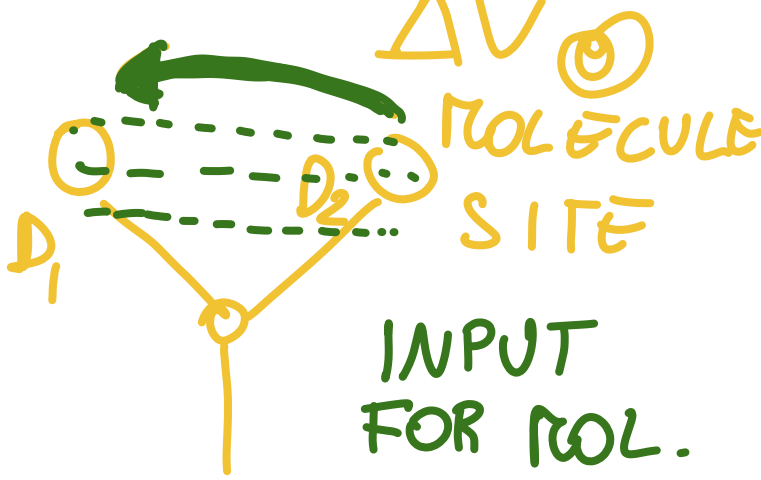

→ SIZE WIRE

→ CRISTAL ORG → SAM ON THE PATTERNED WIRE

→ DIFFICULT CONTROL OF RESOLUTION

# 2.3) INPUT / CLOCKING (external influence)

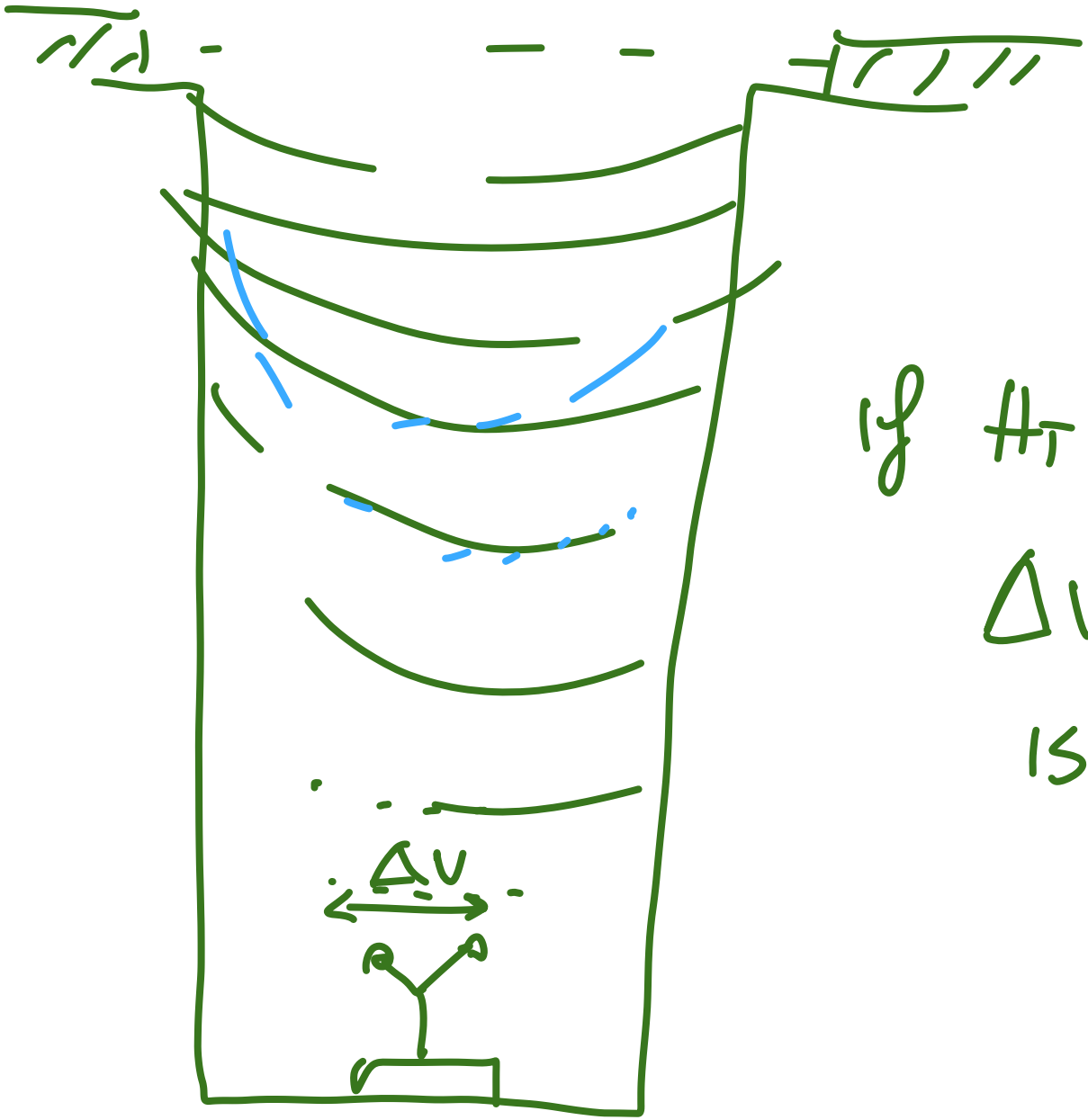



MAXIM. > $H_T$ > $H_M + H_W$ ← CLOCKING

ΔV IS USEFUL @ MOL. SITE

$H_T < H_{T\,MAX}$ ! $\Delta V$ ACROSS D1-D2 SUFFICIENT FOR POLARIZATION

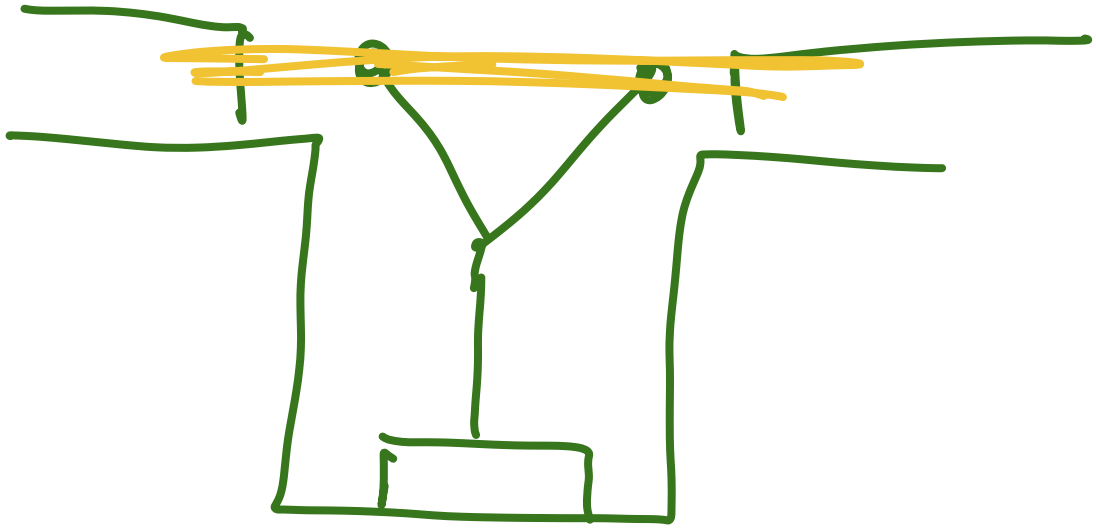



if $H_T$ is too HIGH

$\Delta V$ @ TOL SITE

IS TOO SMALL

$H_T < H_{MIN}$ : ELECTRODES USED FOR CLOCK →



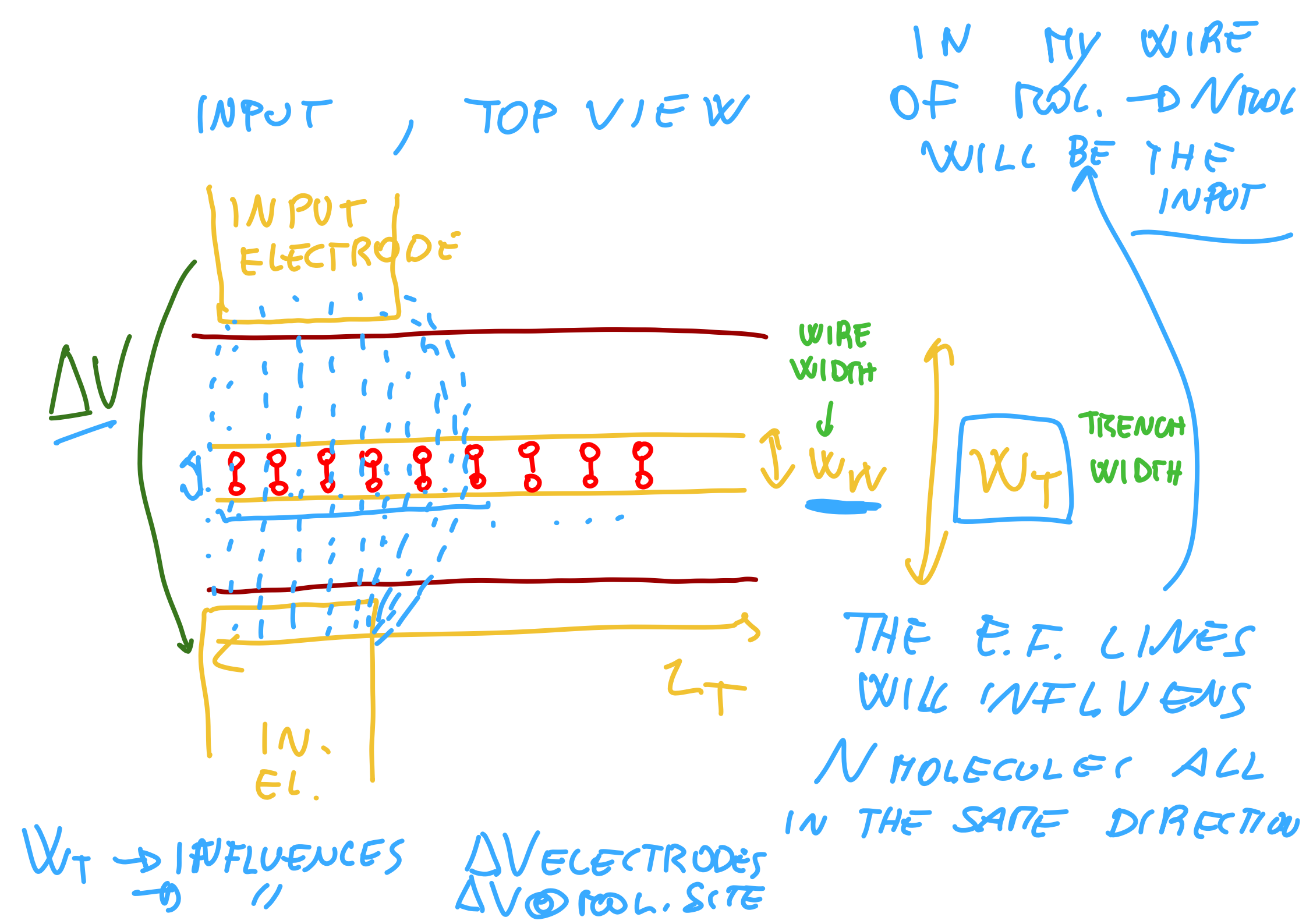
if $H_T$ is SMALL

$\Delta V$ @ POL SITE

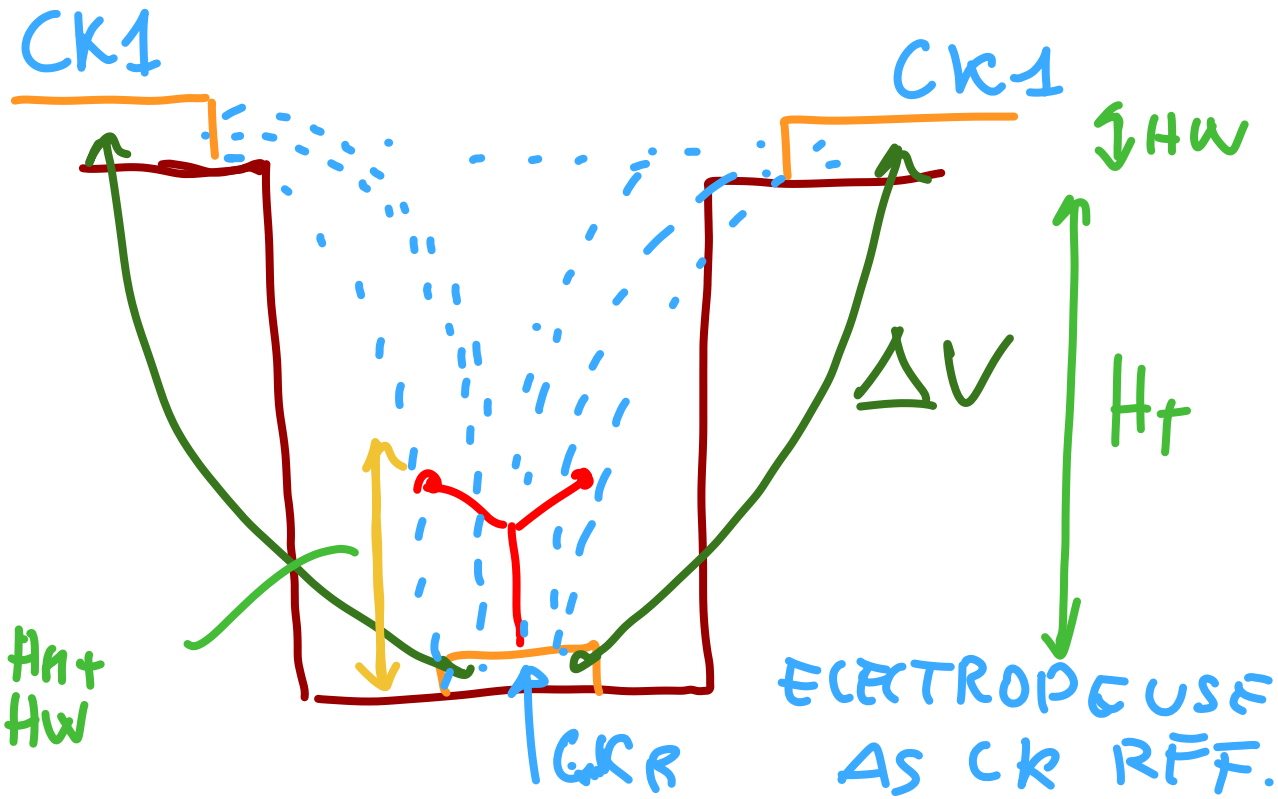
GOOD

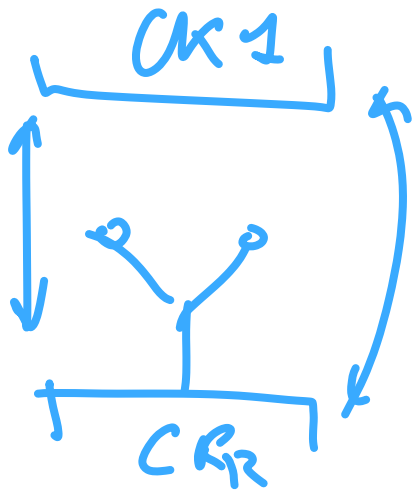
GOOD FOR INPUT

NOT GOOD FOR CK →


INPUT , TOP VIEW
IN MY WIRE OF MOL. → N MOL WILL BE THE INPUT
INPUT ELECTRODE
ΔV
WIRE WIDTH
$W_W$
$W_T$
TRENCH WIDTH
$L_T$
IN. EL.
THE E.F. LINES WILL INFLUENS N MOLECULES ALL IN THE SAME DIRECTION
$W_T$ → INFLUENCES → // ΔV ELECTRODES
ΔV @ MOL. SITE

# CLOCKING



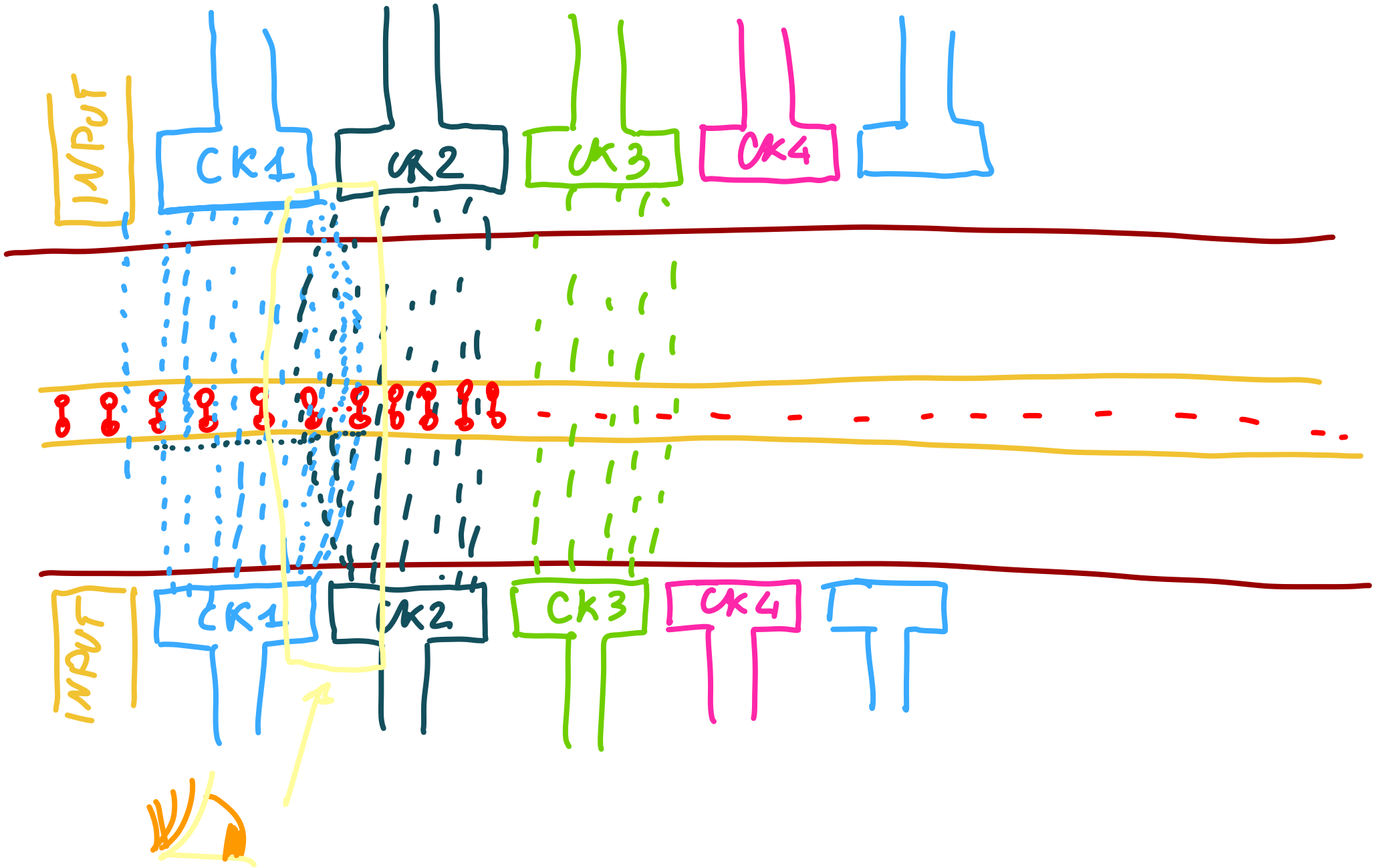



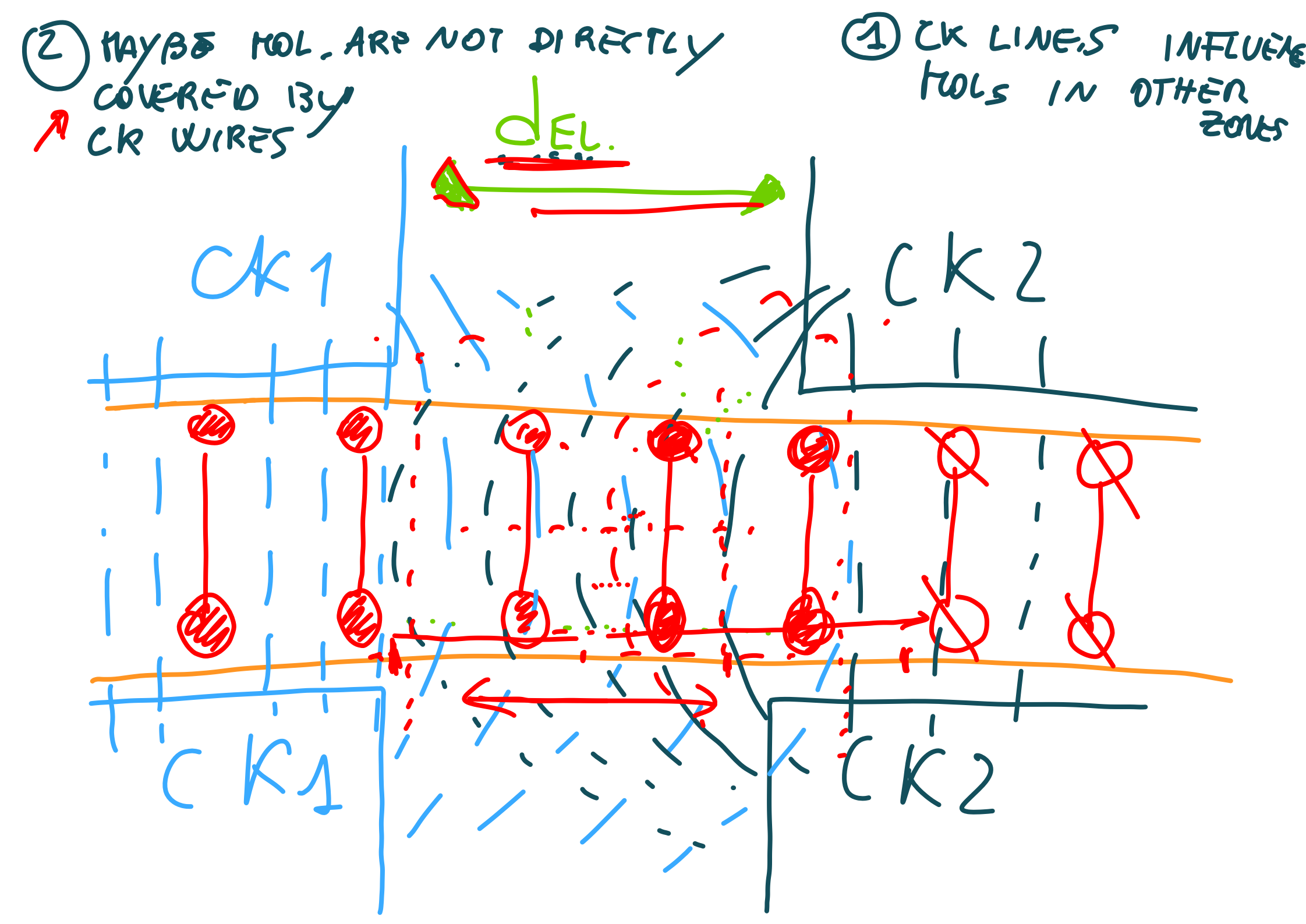

IDEAL CLOCK DISTRIBUTION VERY DIFICULT

IF $H_T$ IS ENOUGH THE E.F. LINES @ POL SITE ARE VERTICAL, UNIFORM ⟶ CAN BE USED AS CK

$$H_T = \alpha (H_M + H_W)$$

# TOP VIEW CLOCKING FOR PHASE ORGANIZATION




(2) MAYBE MOL. ARE NOT DIRECTLY COVERED BY CK WIRES
(1) CK LINES INFLUENCE MOLS IN OTHER ZONES
DEL.
CK1
CK2
CK1
CK2

THE PHASE SEQ.

| CK1 | CK2 |
| --- | --- |
| NO CK | NO CK |
| CK APPLIED | NO CK |
| CK APPLIE | APPLIED |

(2) CK1 + CK2 ON CREATE CONSTRUCTIVE INTERFERENCE

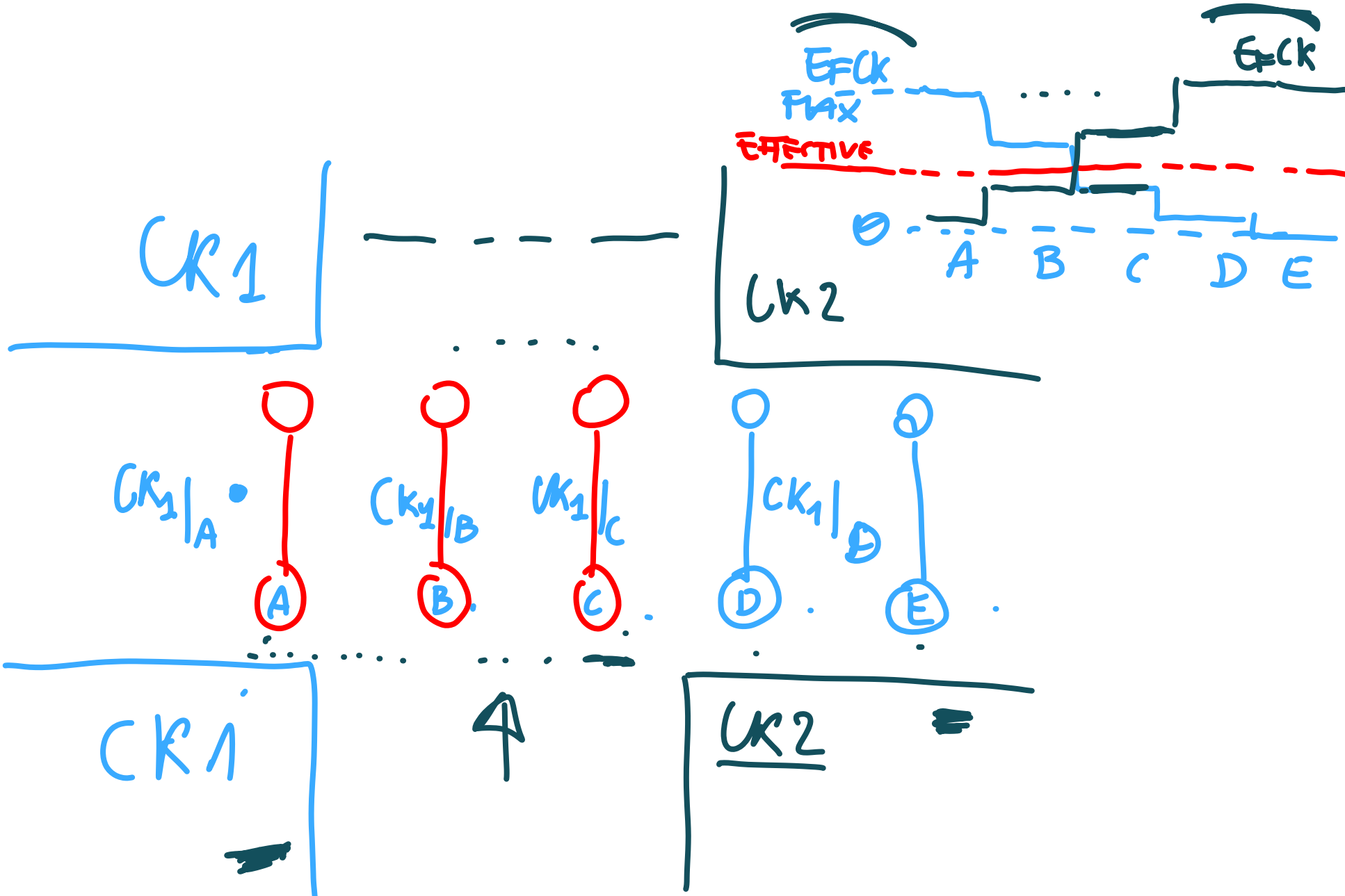
ALSO FCOL. BW ELE. ARE INFLUENCED

→ depl. < MAXd : CONSTR. INT. TRUE

(1) NOT A REAL PROBLEM IN WIRE

→ INFO PROPAGATES IN A WAVE

THE LIMIT OF INFO IS NOT CORRESPONDENT TO GEOMETRICAL LIMIT OF CK. ELECTRODE


EFCK
FMAX
EFFECTIVE
A
B
C
D
E
CK1
CK2
CK1|A
CK1|B
CK1|C
CK1|D
A
B
C
D
E
CK1
4
CK2

# PROCESS VARIATIONS - PARAMETERS

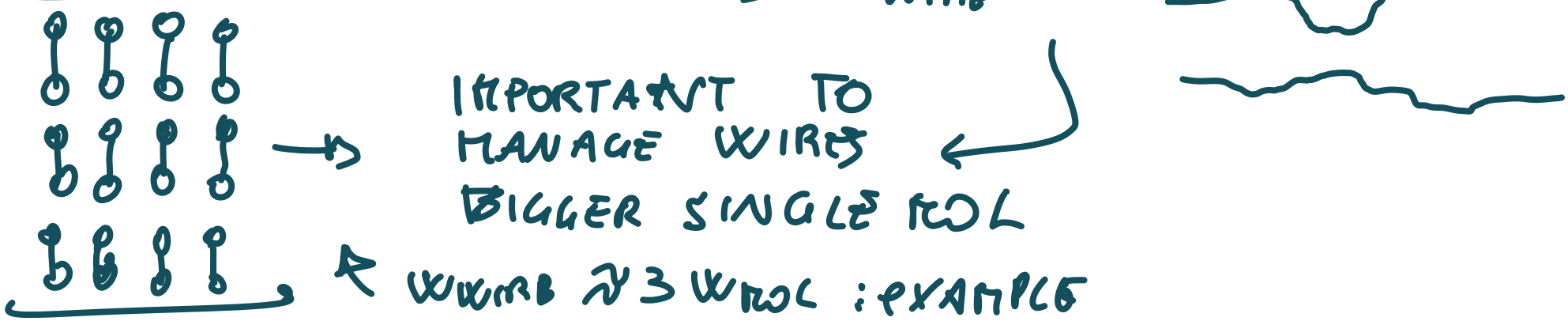
## PARAMETERS FROM TECH.

- MOLECULE : → SYNTHESIS
  - → SIZES NOW UNIFORM
  - → 1 DOT MISSING
  - → 1-2 ATOMS MISSING

- SAM : - REGIONS FORMED, NOT NECESSARILY REGULAL IN ALL THE PATTERNED STRUCTURE

BUS OF MOL — SUBSTRATE

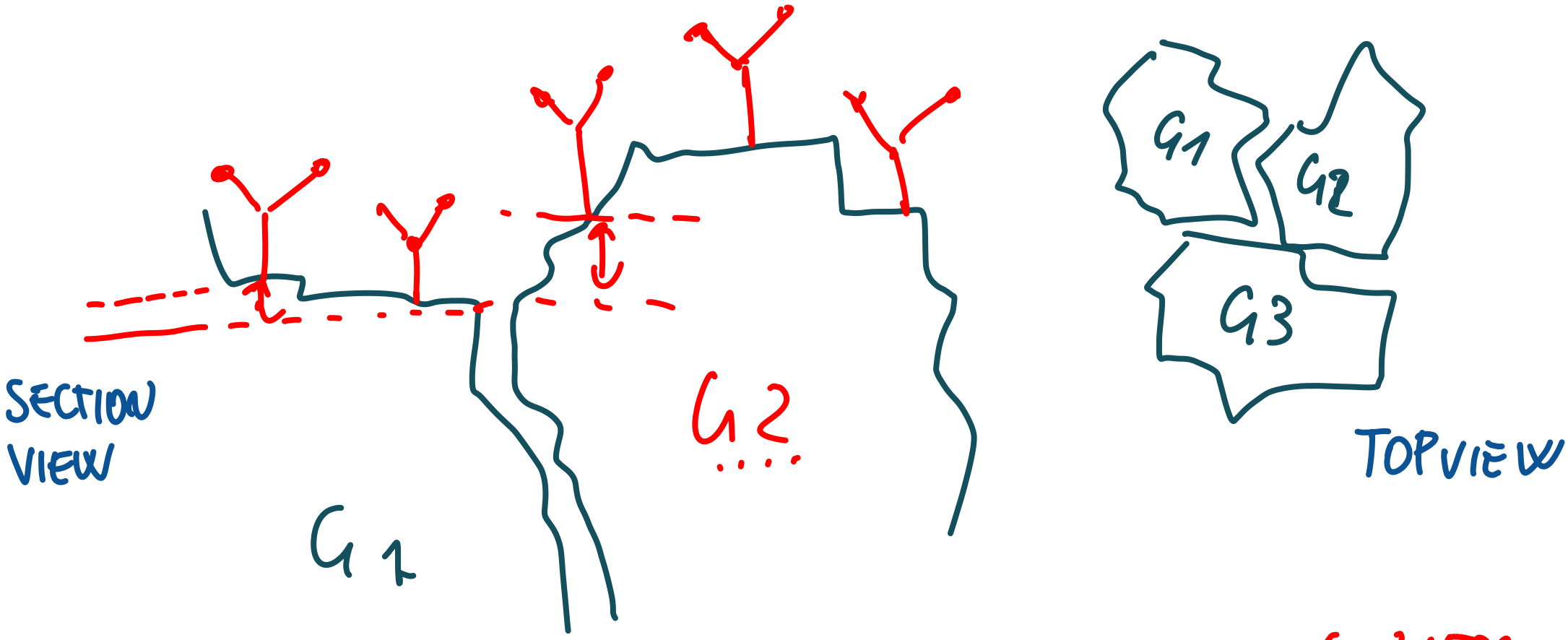
→ W WIRE → NOT REGULAR



IMPORTANT TO MANAGE WIRES BIGGER SINGLE MOL

↑ NUMBER OF 3 MOL : EXAMPLE

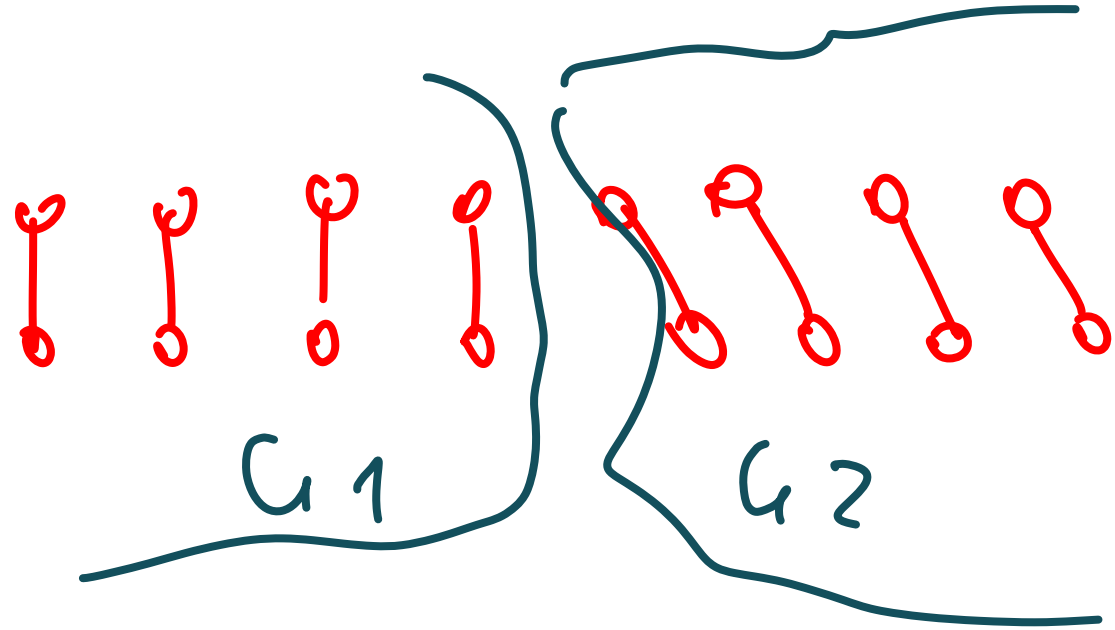
# GUIDING WIRE CRISTAL STRUCTURE - PARAMETERS



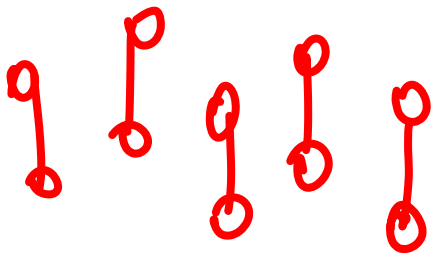

- DIFFERENT H. WITHIN EACH GRAIN (INTRA GRAIN)

(VERTICAL DISPLACEMENT OF ROI.)

- ALONG GRAINS (INTER GRAINS)

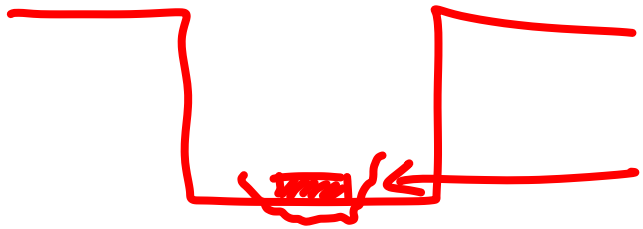



TILT DUE TO GRAIN ORIENTATION



SHIFT DUE TO ANCHORING POINTS NOT IDEAL

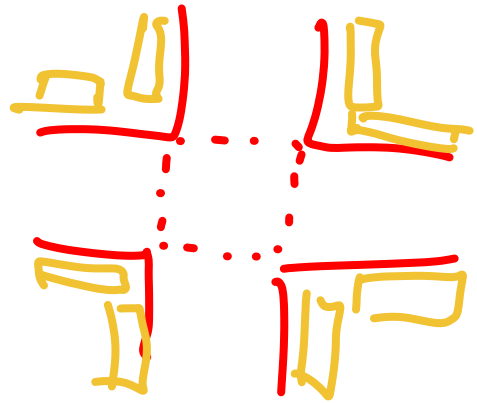
- TRENCH PARAMETERS . $H_T$, $W_T$



FLATNESS OF TRENCH.

- ELECTRODE PARAMETERS – DISTANCE BW-ECECTRON.

↳ HOW TO DEAL WITH CORNERS



# CRISTALLIZATION

1) STRUCTURE IDENTIFIED

2) PARAMETERS ENTANGLED
BW TECH - DEVICE - FUNCTIONALITY

3) MOLECULAR DYNAMICS SIMULATION
FOUNDAMENTAL TO STUDY AND
GUIDE THE FABRICATION PROCESS

→ THE TREND IN FUTURE NANOELECTRONICS