

EPFL



MICRO-435
Quantum and
Nanocomputing

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MOLECULAR FCN TECHNOLOGY

OBJECTIVES

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

- SINGLE MOL. EXPECTED
FUNCTIONAL BEHAVIOR
(MODELING)

- MOLECULES IN
THE SYSTEMS
FUNCTIONAL
BEHAVIOR
(MODELING)

THE MOLECULE

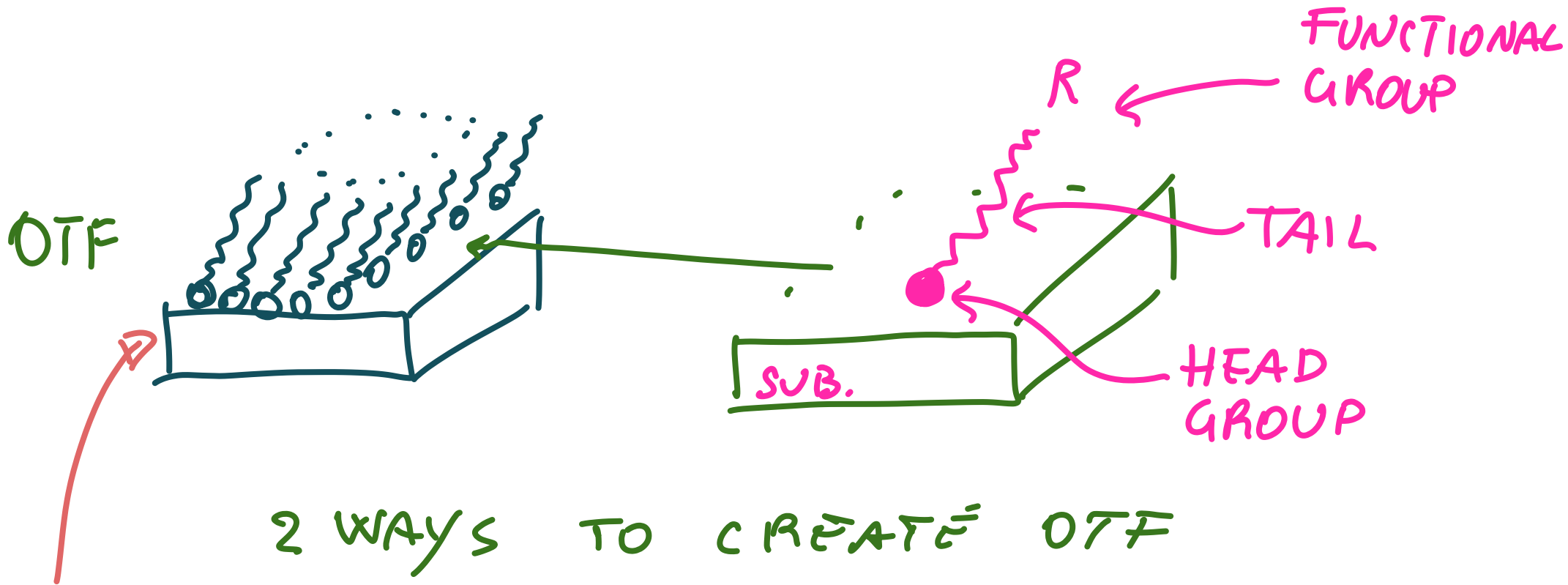
SYNTHESIS
FEASIBILITY
AND YIELD

FABRICATION
- ORGANIC
THIN FILMS
- WIRINGS FOR
MOL. BIASING

COMPUTATIONAL
CHEMISTRY
ANALYSIS

POSSIBILITY
TO OBSERVE / MEASURE
TESTABILITY

BRIEF SUMMARY ON ORGANIC THIN FILMS - OTF



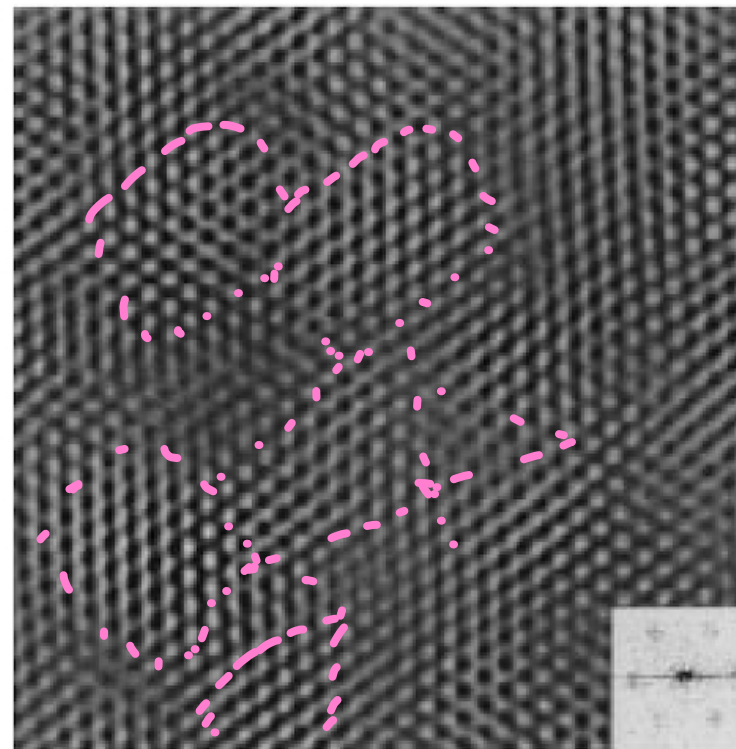
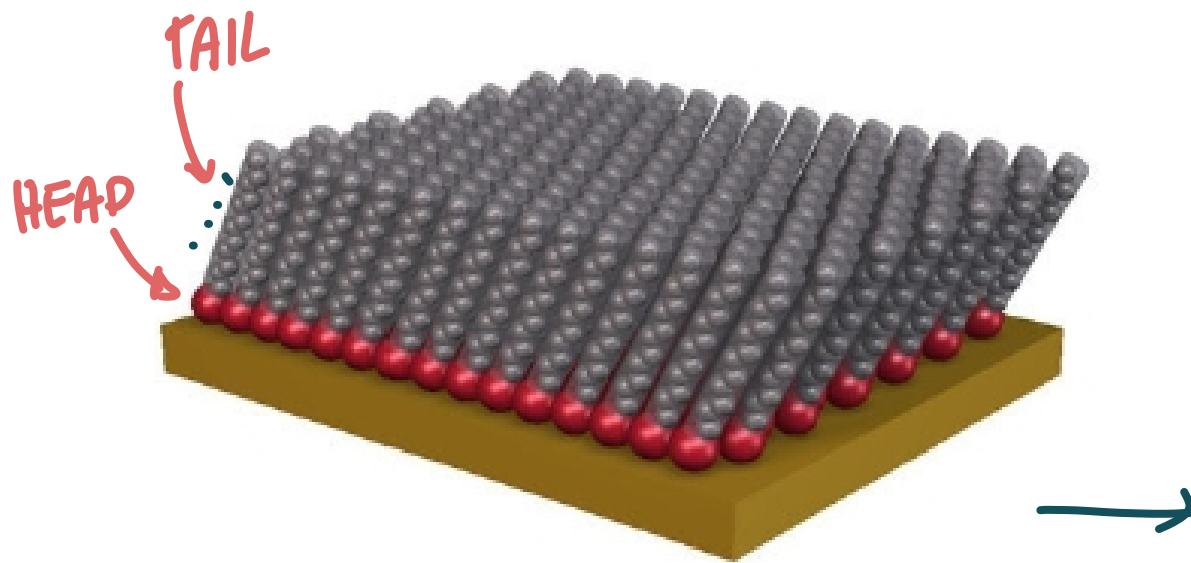
2 WAYS TO CREATE OTF

DENSE
PACKED
SELF
ORGANIZED

→ LANGMUIR LAYER

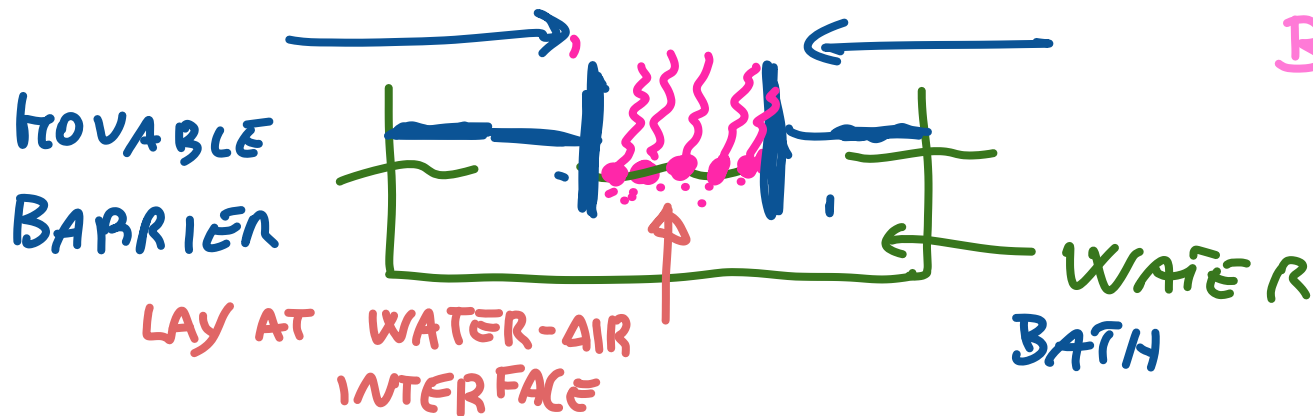
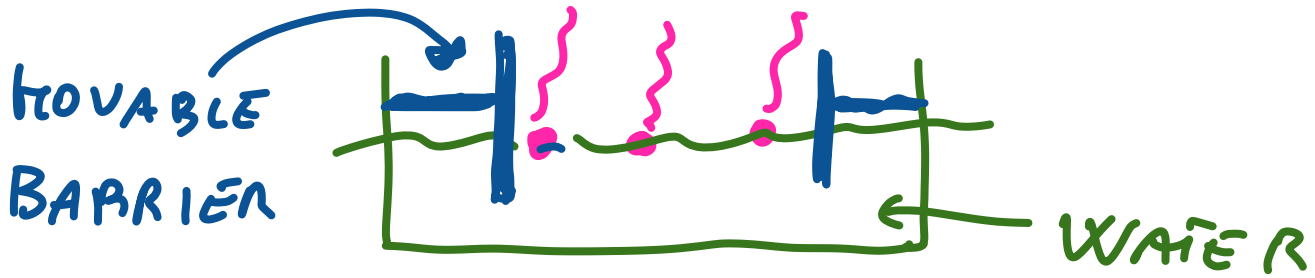
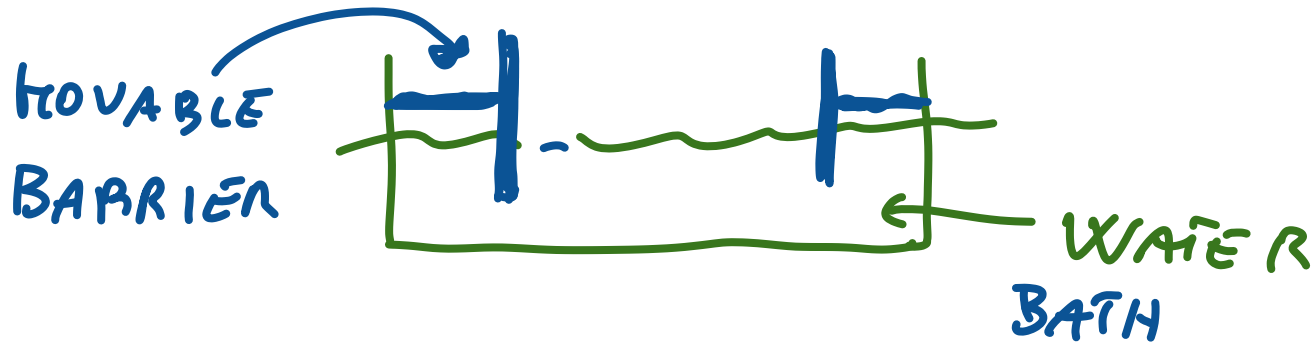
→ SELF-ASSEMBLY MONOLAYER-SAM

OTF EXAMPLE



THIOL OTF - REGULAR
ORIENTATION IN SUBZONES

LANGMUIR LAYER



REGION
HYDROPHOBIC

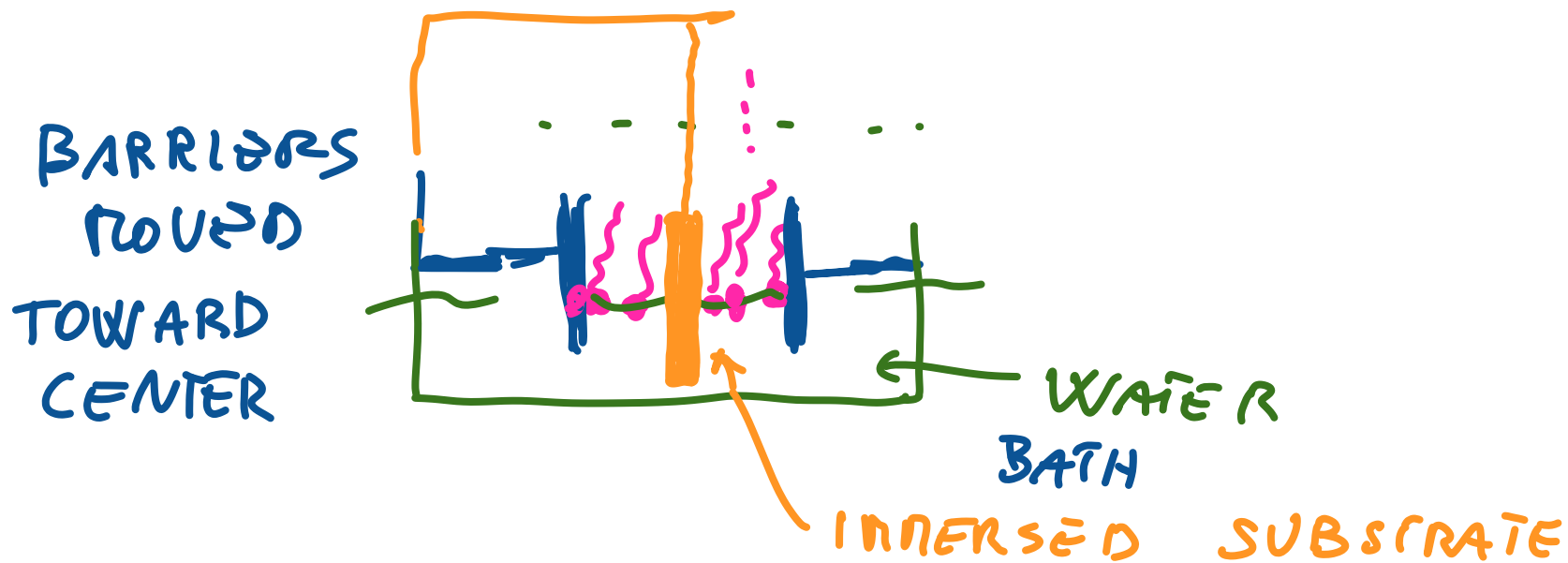
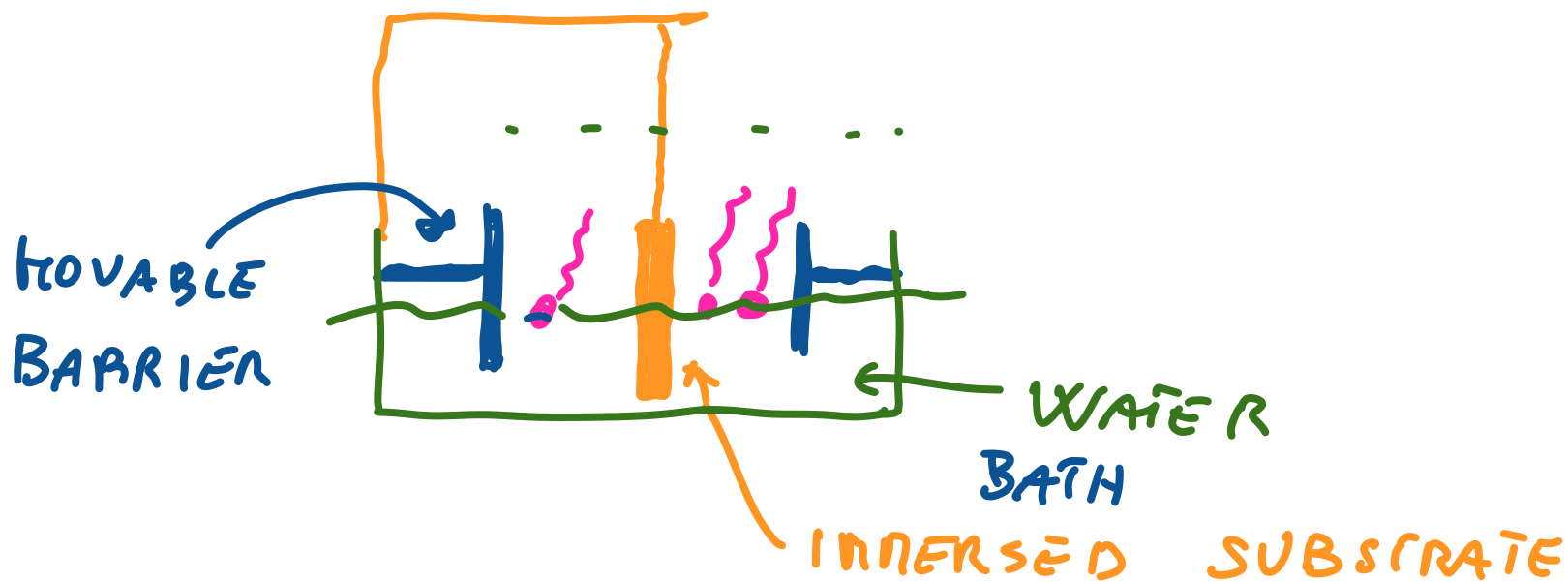
●
HYDROPHILIC
REGION

MOLECULES DEPOSITED
WITH A GIVEN
CONCENTRATION

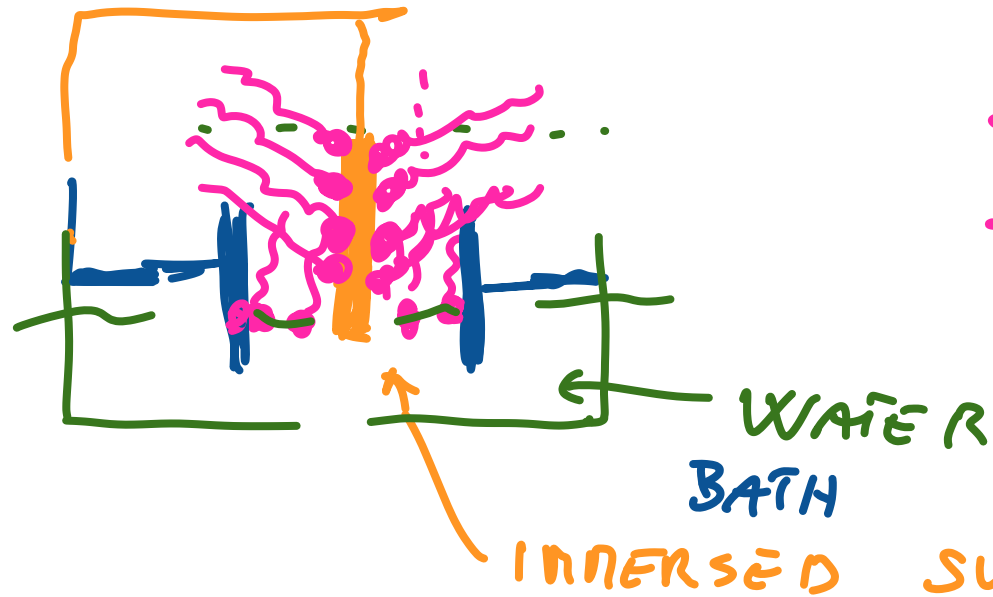
BARRIERS MOVED
TOWARD THE
CENTER

FILM CREATED

LANGMUIR-BLODGETT (LB)



SUBSTRATE IS
PULLED



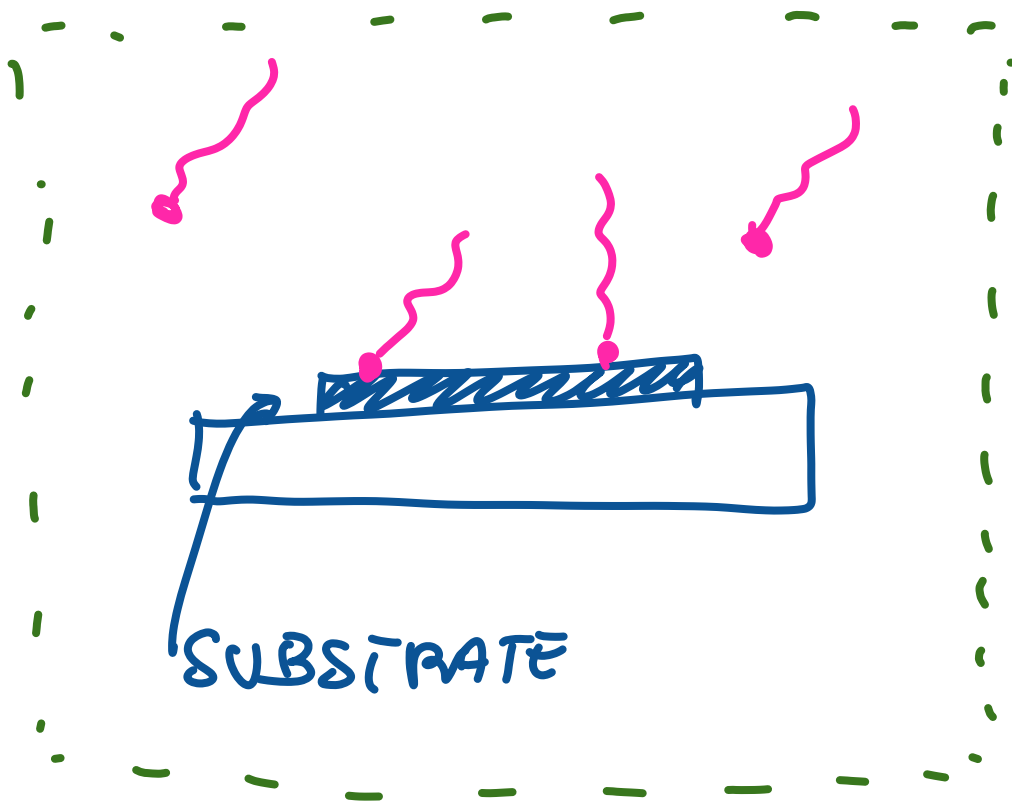
BARRIERS
SQUEEZED
→ CENTR

MOLECULES ATTACH IN A
IN A REGULAR ORGANIZATION

THE PROCESS CAN BE ITERATED TO OBTAIN MULTILAYER
LB FILMS

SAM - SELF ASSEMBLED MONOLAYERS

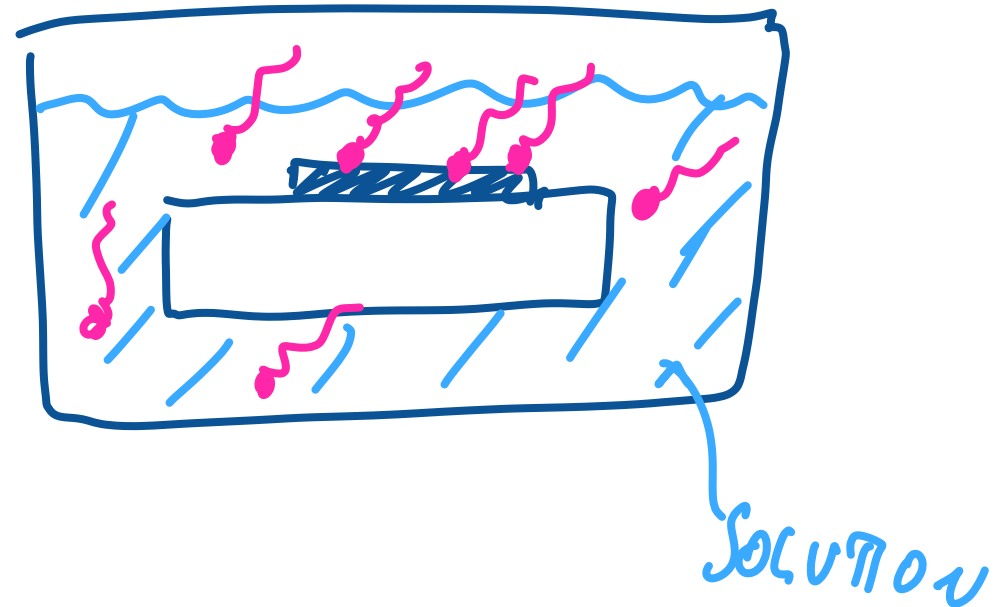
VAPOR



SUBSTRATE

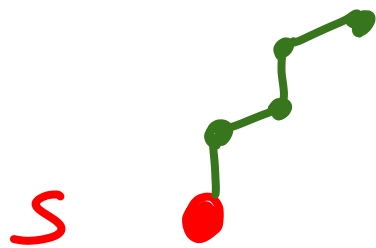
SPONTANEOUS ADSORPTION OF
MOI ON SUB. VIA
CHEMICAL BOND CREATION

LIQUID

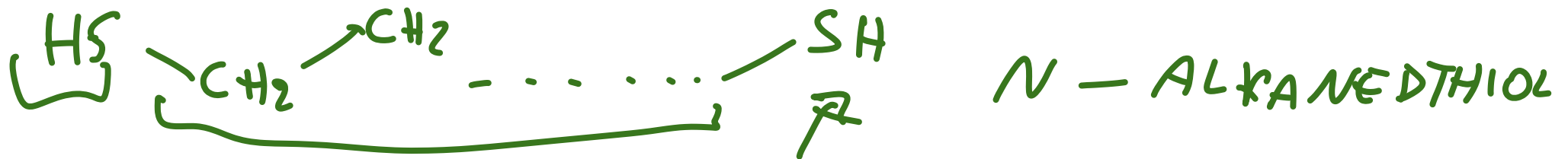
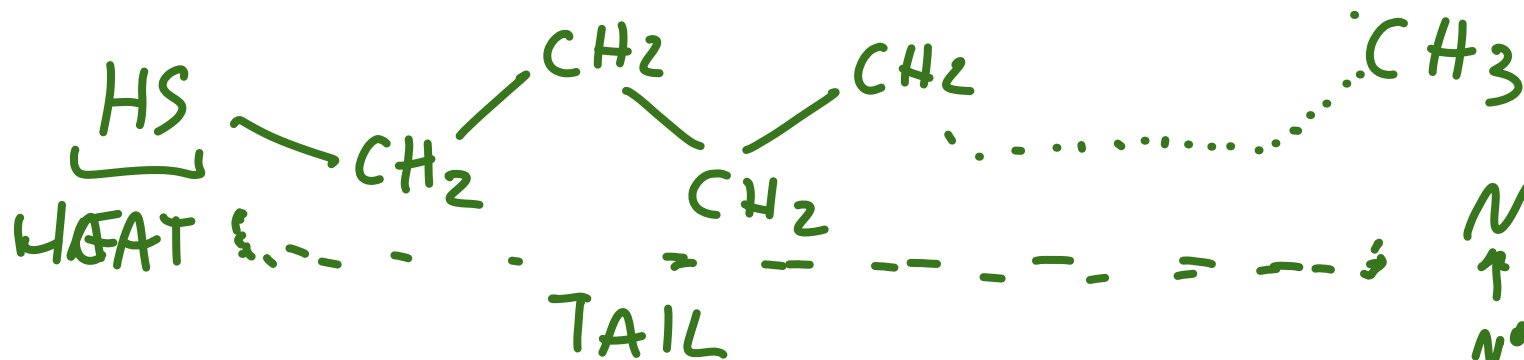


SOLUTION

EXAMPLE: GOLD + SULFUR



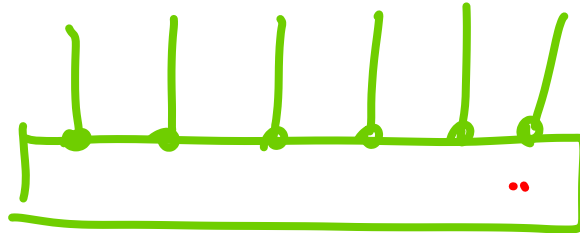
THIOL -SH



..... many others are possible and used

FOR BISFERROCENE RECIPE 2 STEPS

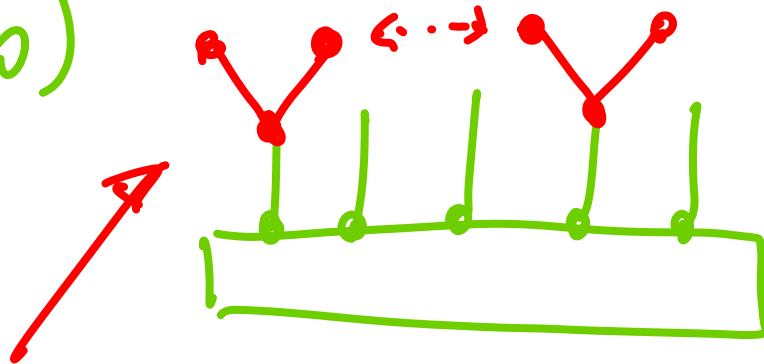
a)



SAM WITH THIOLS

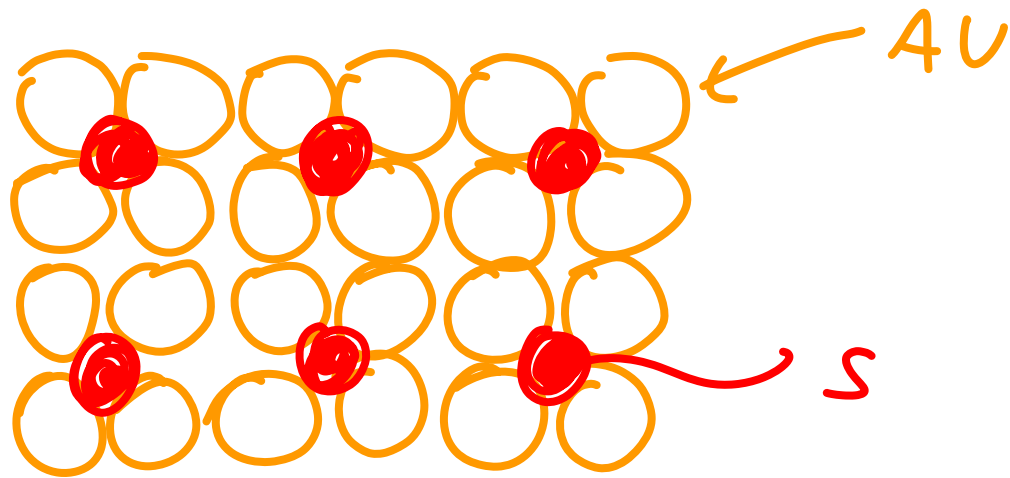
- PROPER CONCENTRATION
- " GOLD LATTICE ORIENTATION

b)



BISFERROCENE + THIOLS

HINDRANCE OF
BISFERROCENES

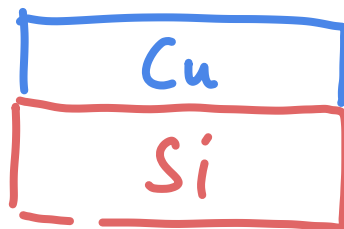


TYPICAL
ATTACHMENT
(TOP VIEW)

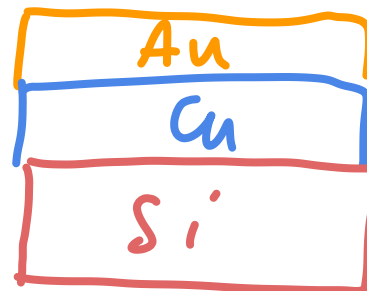
SIMULATION OF THE PROCESS (LAMPS) USING MOLECULAR DYNAMICS



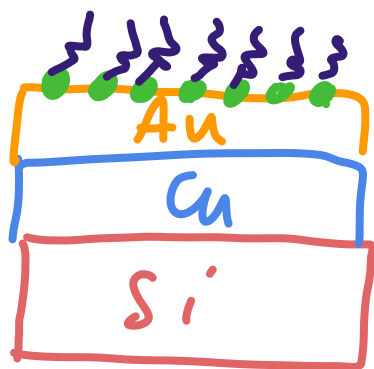
SUBSTRATE



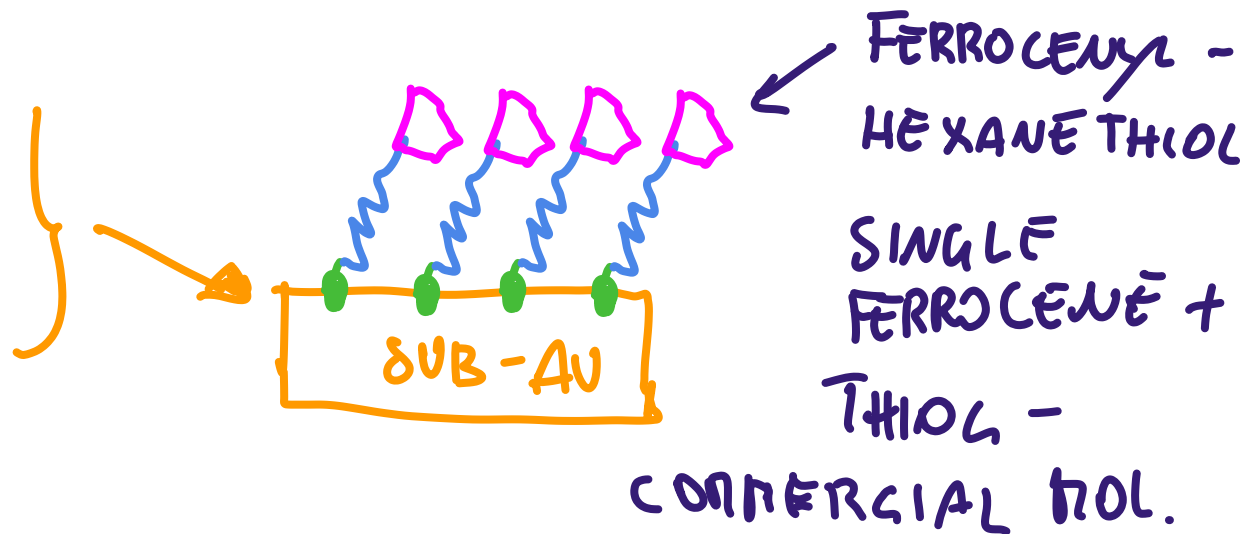
COPPER LAYER



GOLD

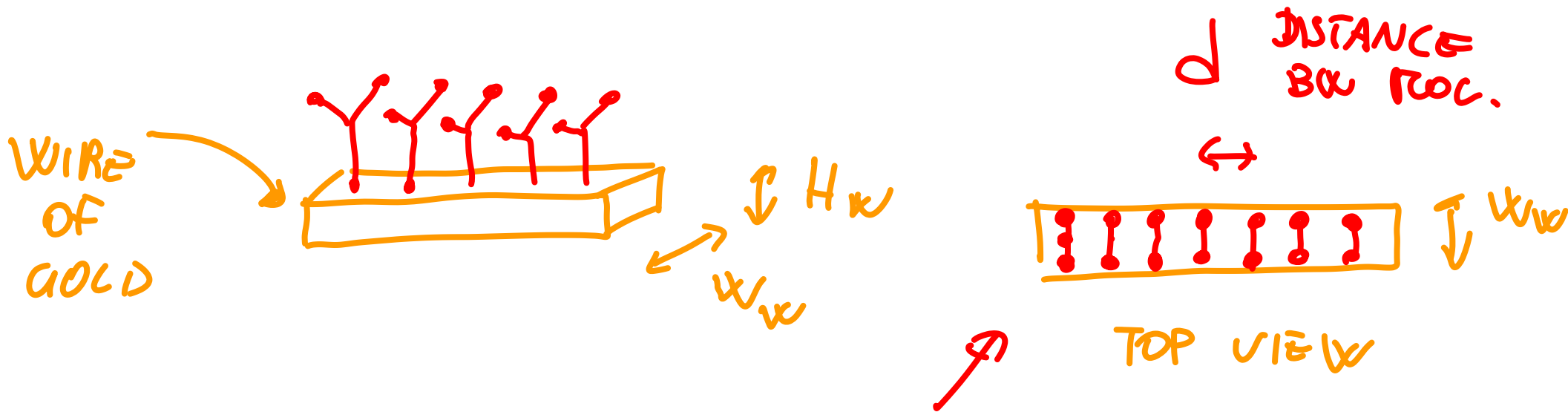


THIOLS



2) THE MOL-FCN STRUCTURE

2.1) THE MOL-FCN WIRE (GUIDING WIRE)



TOP VIEW
ORGANIZATION

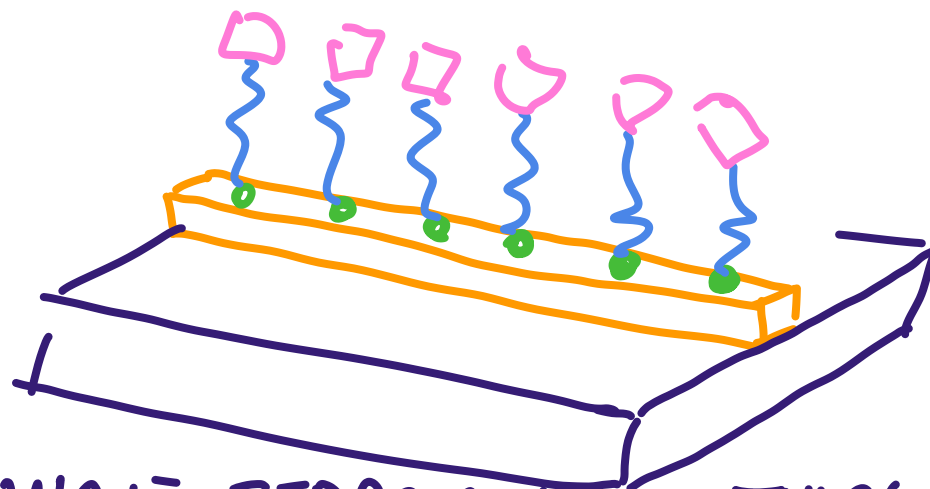
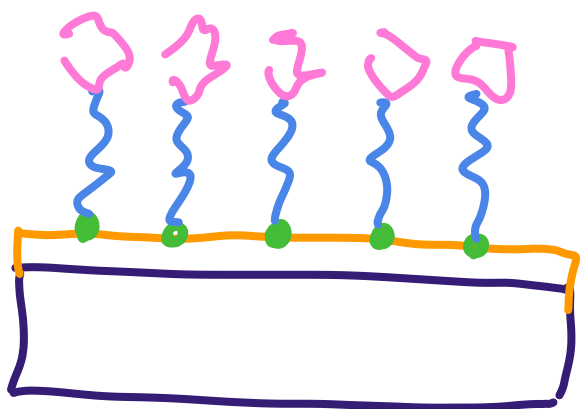
DEPENDS

→ GOLD STR.

→ SH → ATTACHMENT

→ BIF. HINDRANCE

MOLECULAR DYNAMICS SIMULATION

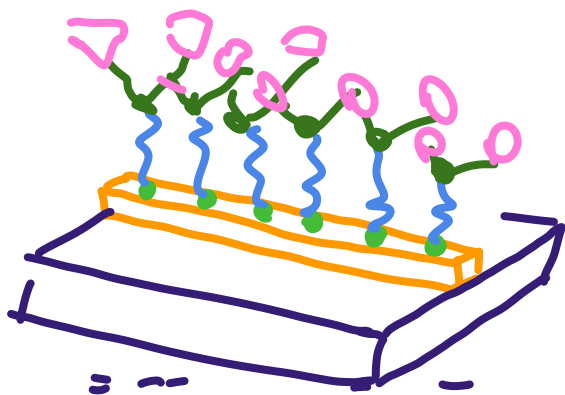


GOLD WIRE + SINGLE FERROCENE + THIOL

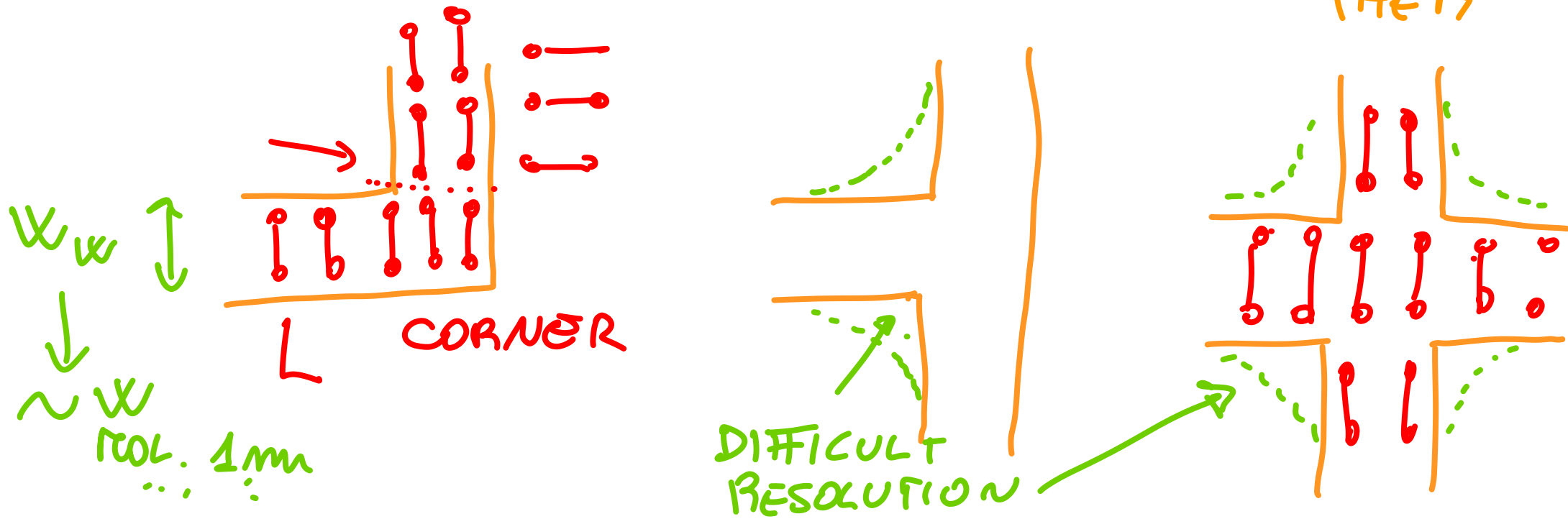
- OXIDIZED - NO VERTICAL CLOCK

- OXIDIZED + VERTICAL CLOCK

- BISFERROCENE-THIOLATED + V. CLOCK



2.2.) MORE COMPLEX PATTERNS & MOLECULES DEPOSITION ON THEM

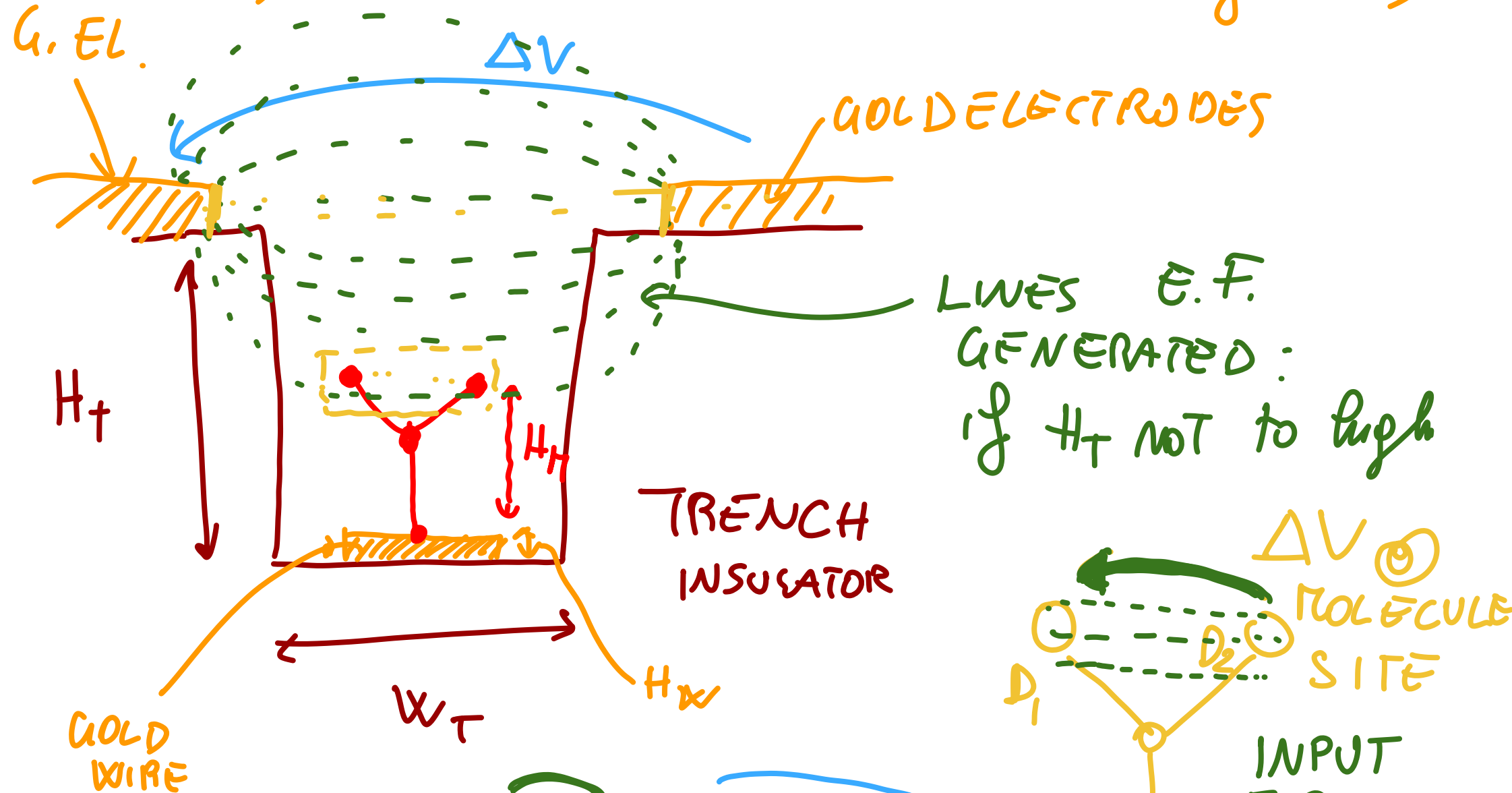


→ SIZE WIRE

→ CRISTAL ORG → SAM ON THE PATTERNED WIRE

→ DIFFICULT CONTROL OF RESOLUTION

2.3) INPUT / CLOCKING (external influence)

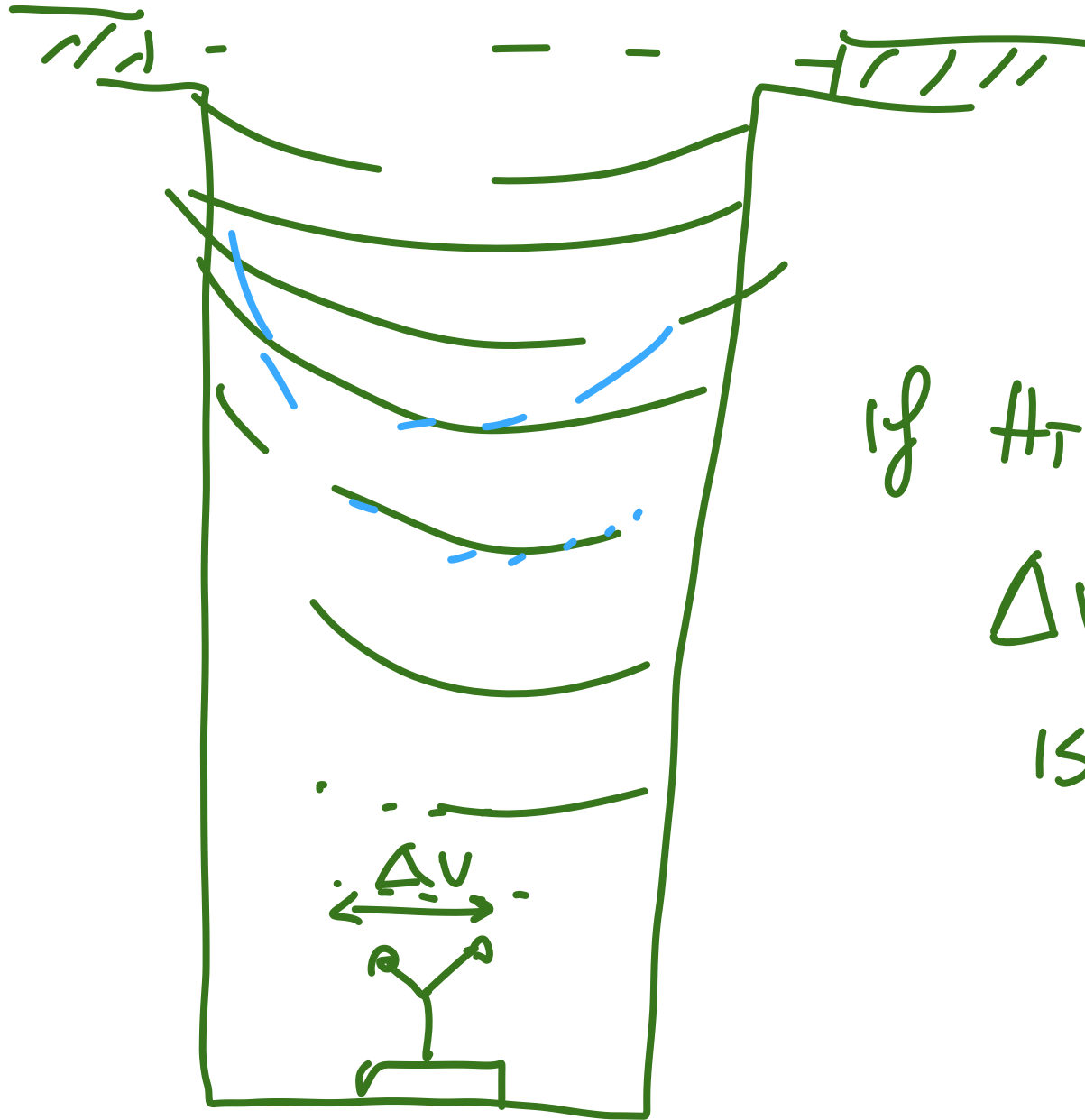


MAXIM. $\Delta V > H_T > H_M + H_W$
 ΔV IS USEFUL @ MOL. & CRE

CLOCKING

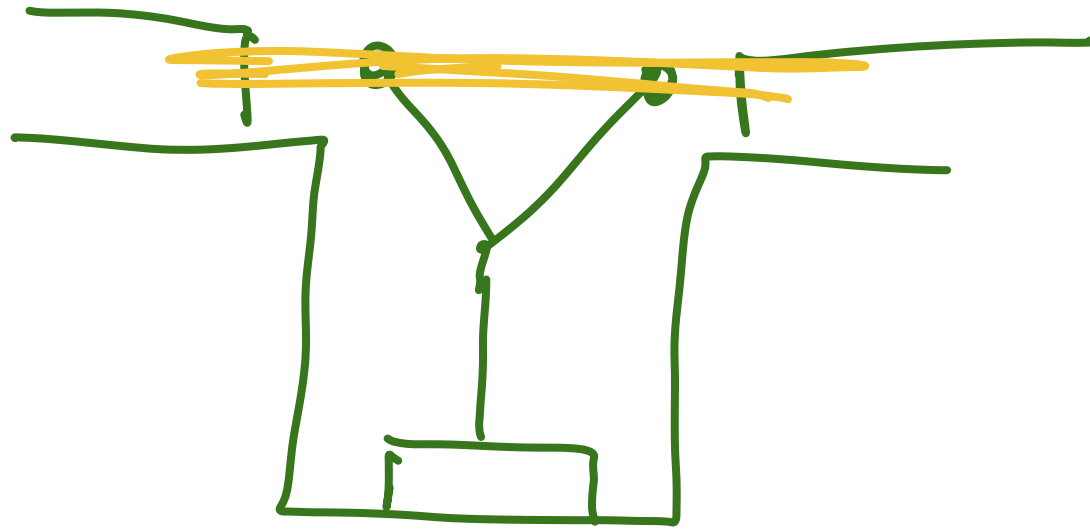
INPUT FOR MOL.

$H_T < H_{TMAX}$! ΔV ACROSS D1-D2
SUFFICIENT FOR
POLARIZATION



if H_T is too HIGH
 ΔV @ TROL SITE
IS TOO SMALL

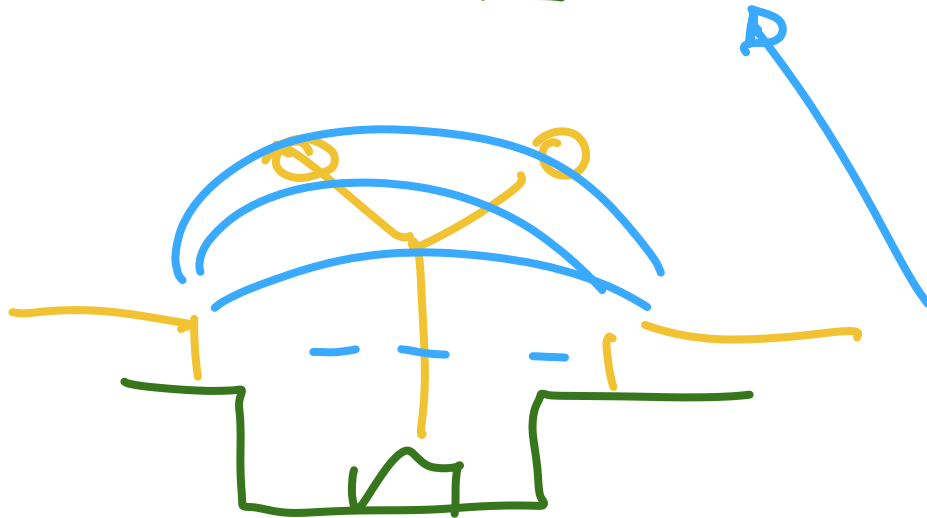
$H_T < H_{MIN}$: ELECTRODES USED FOR CLOCK \rightarrow



if H_T is
SMALL

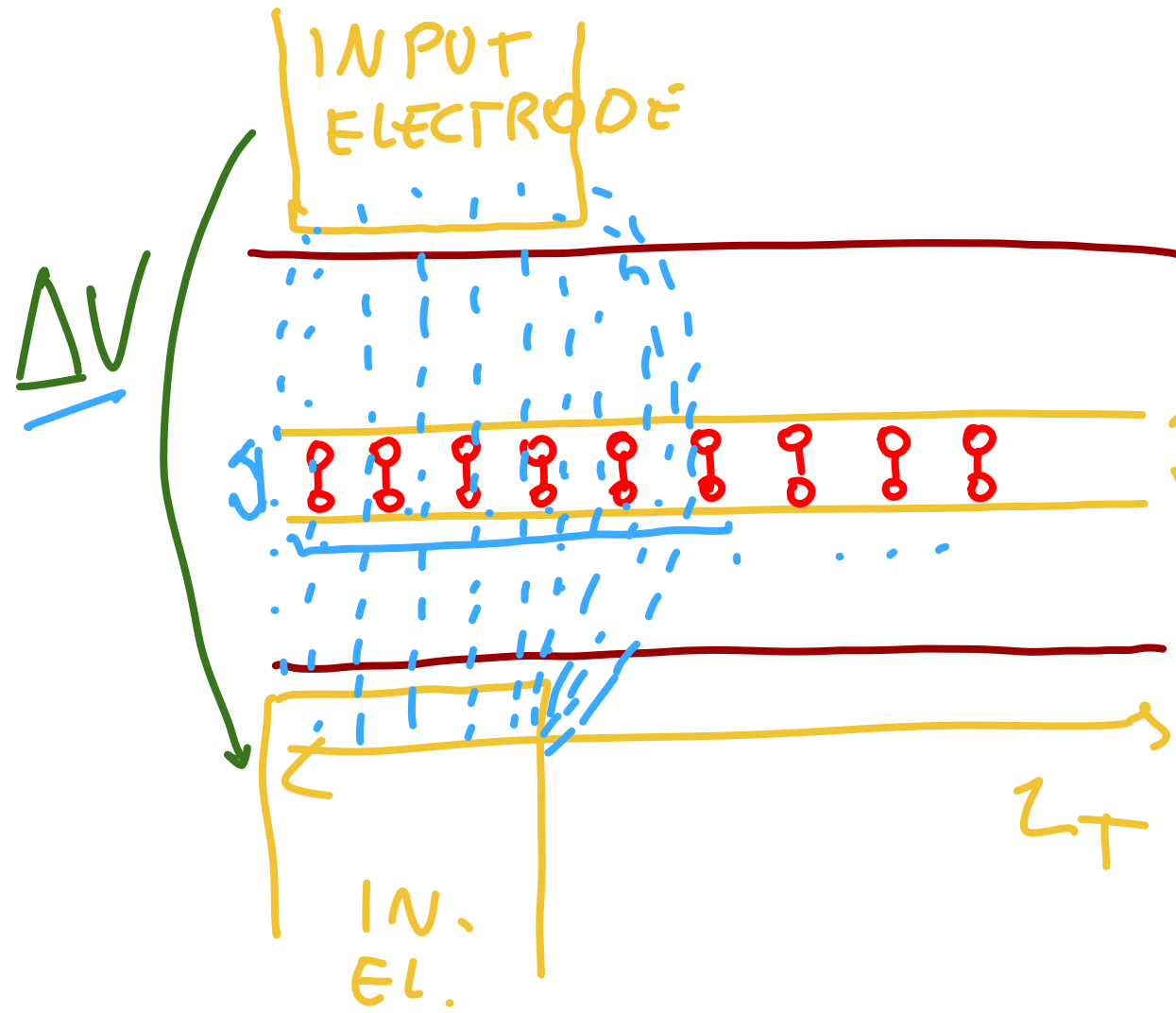
ΔV \odot \oplus FUEL
SITE

GOOD

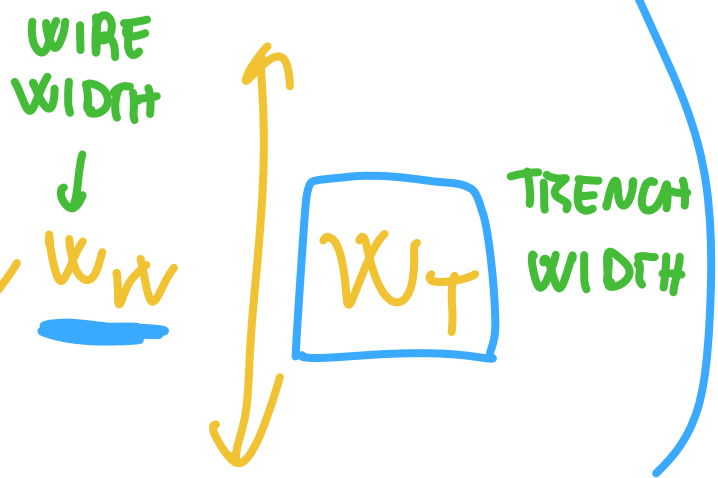


GOOD FOR INPUT
NOT GOOD FOR
CK \rightarrow

INPUT, TOP VIEW



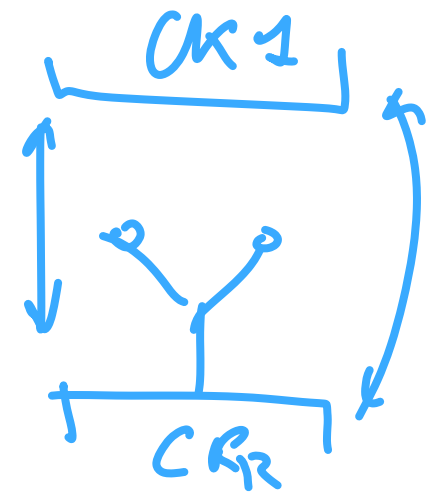
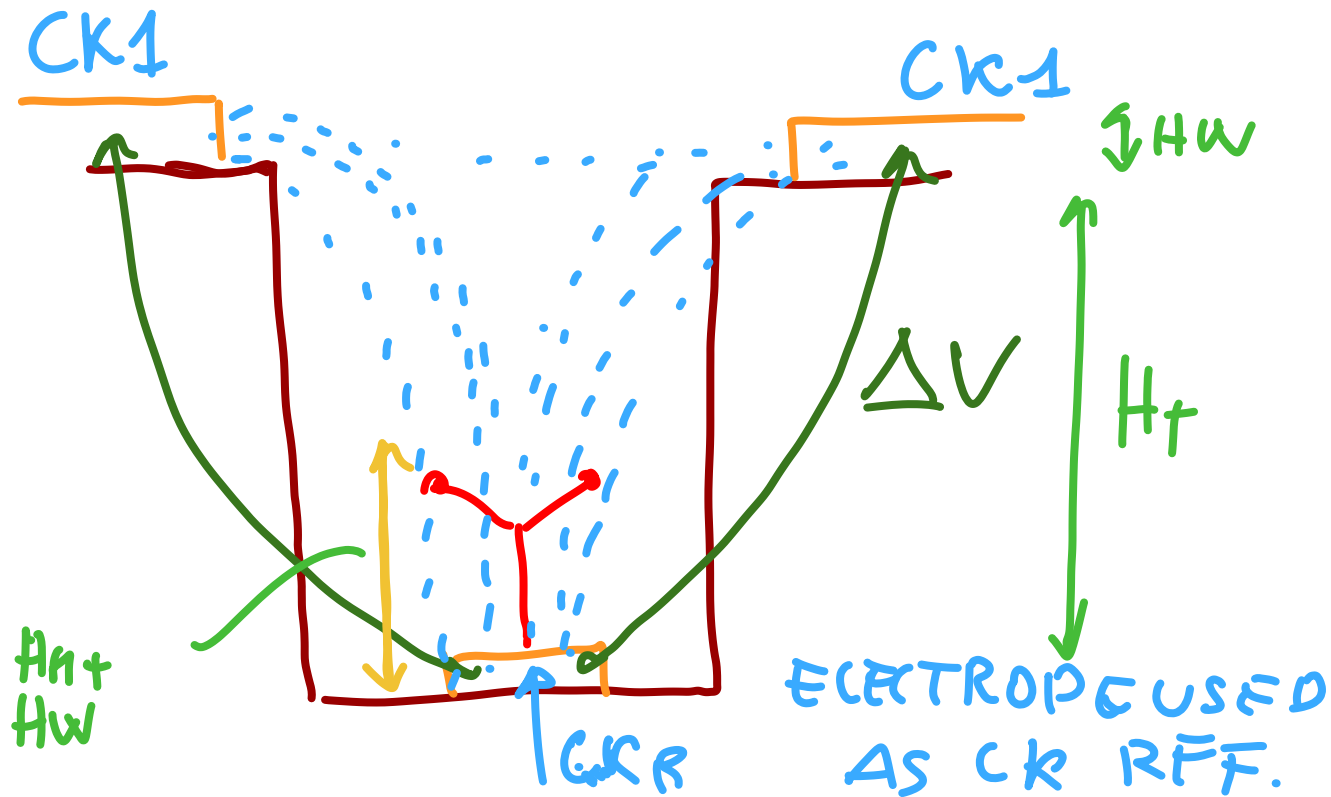
IN MY WIRE
OF POL. → D/POL
WILL BE THE
INPUT



THE E.F. LINES
WILL INFLUENS
N MOLECULES ALL
IN THE SAME DIRECTION

W_T → INFLUENCES
→ " " ΔV ELECTRODES
 ΔV @ MOL. SITE

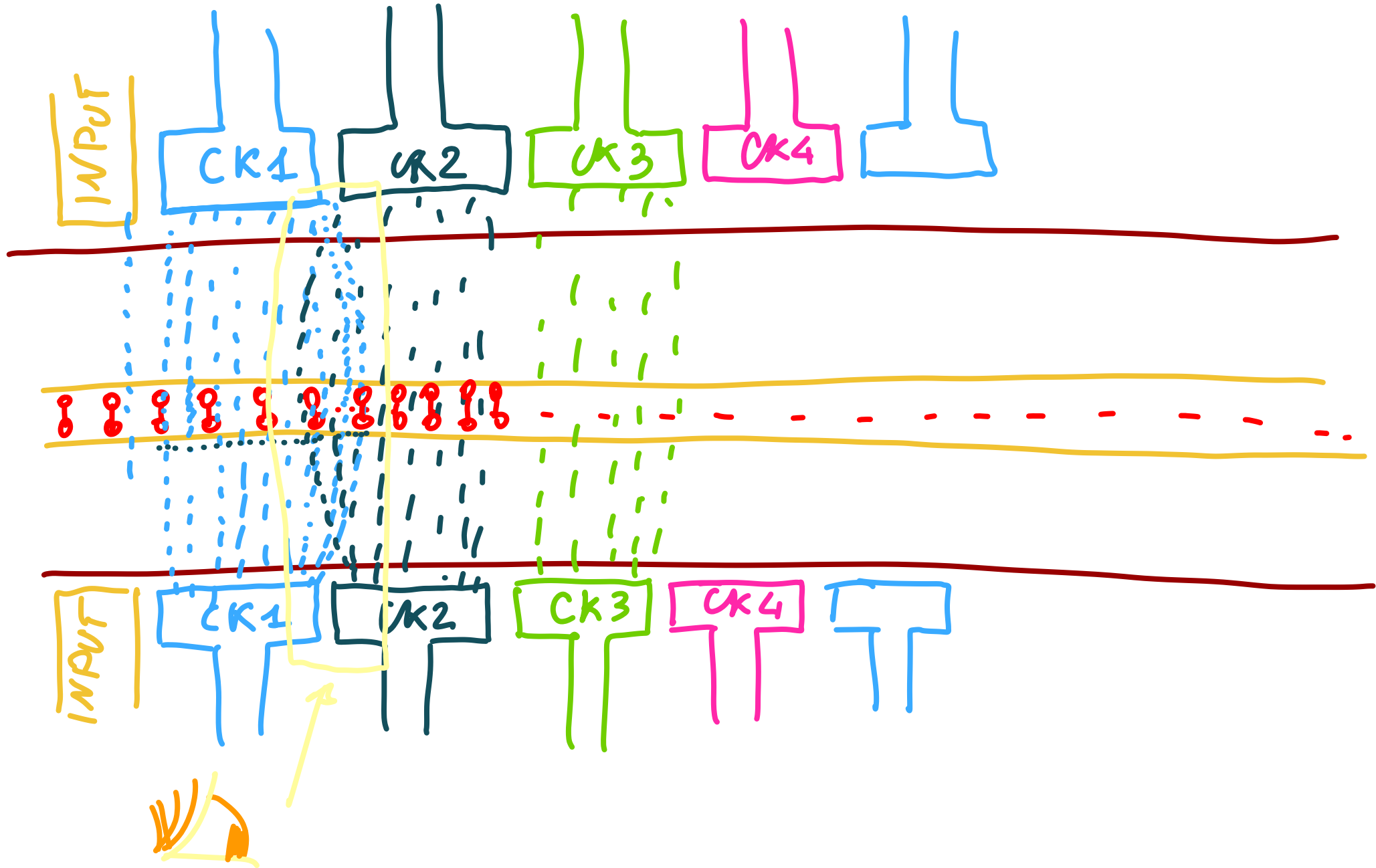
CLOCKING



IDEAL CLOCK DISTRIBUTION VERY DIFFICULT

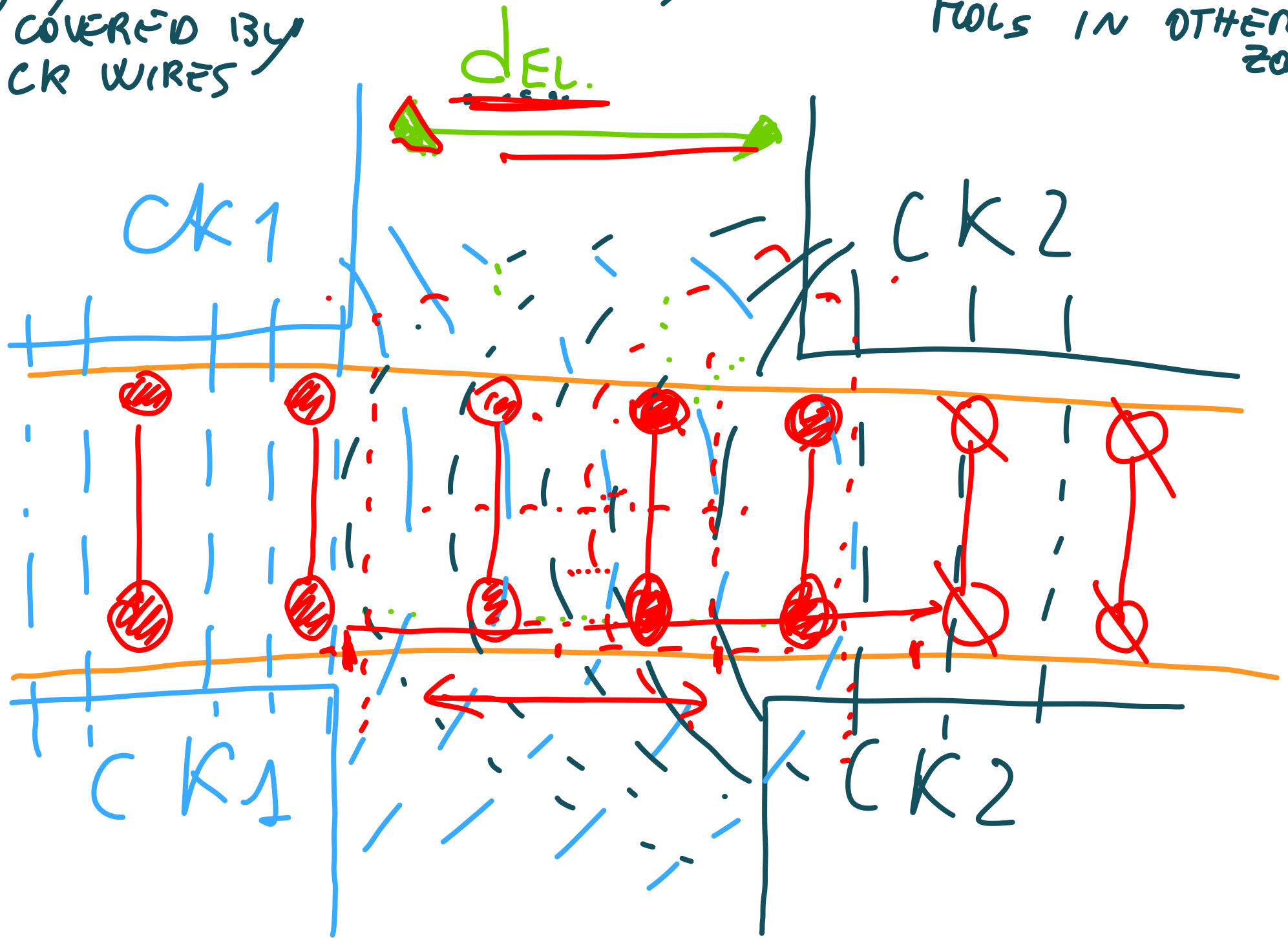
if H_T is ENOUGH THE E.F. LINES @ WELL SITE ARE VERTICAL, UNIFORM \rightarrow CAN BE USED AS CK $H_T = \alpha (H_T + H_W)$

TOP VIEW CLOCKING FOR PHASE ORGANIZATION



② MAYBE MOL. ARE NOT DIRECTLY COVERED BY CK WIRES

① CK LINES INFLUENCE MOL. IN OTHER ZONES

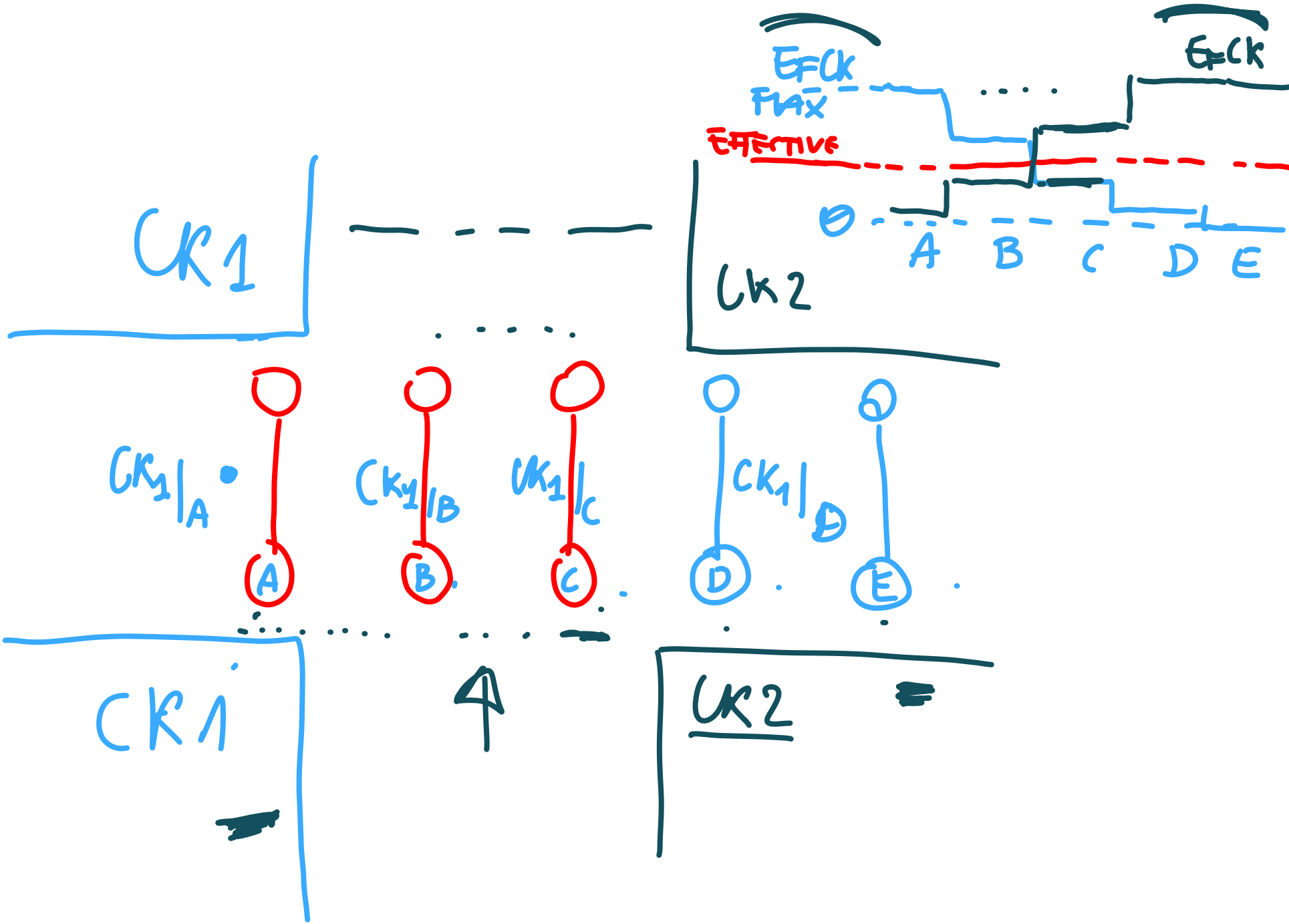


THE PHASE SEQ.

CK1	CK2
NO CLK	NO CLK
CLK APPLIED	NO CLK
CLK APPLIED	APPLIED

② CK1 + CK2 ON
CREATE CONSTRUCTIVE
INTERFERENCE
ALSO TOL. B/W ELE.
ARE INFLUENCED
→ $d_{eff} < \overline{MAX d}$
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



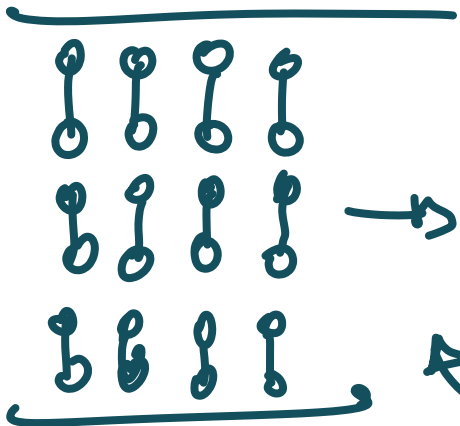
PROCESS VARIATIONS - PARAMETERS

PARAMETERS FROM TECH.

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

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

BUS OF
MOL

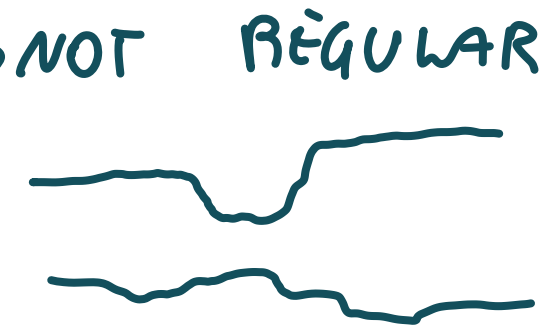


- SUBSTRATE

→ W WIRE

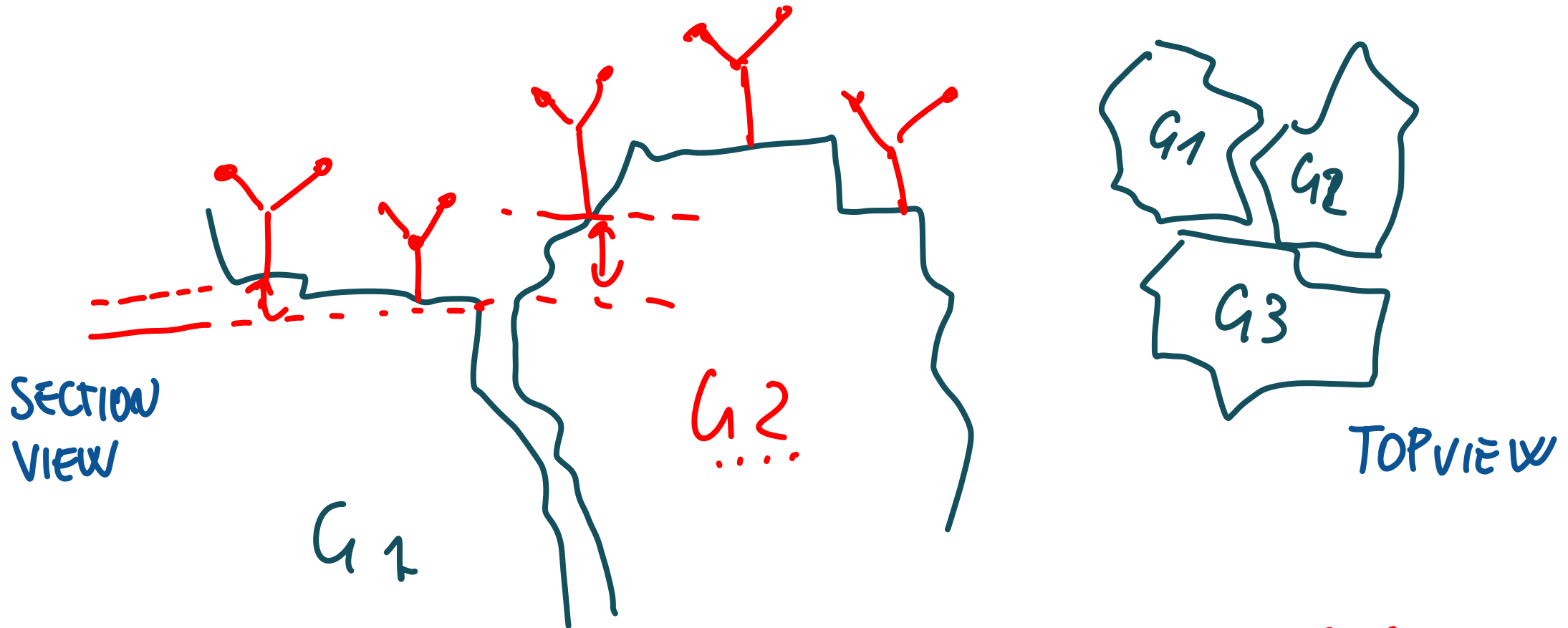
IMPORTANT TO
MANAGE WIRES
BIGGER SINGLE MOL

W WIRE ≈ 3 W MOL : EXAMPLE

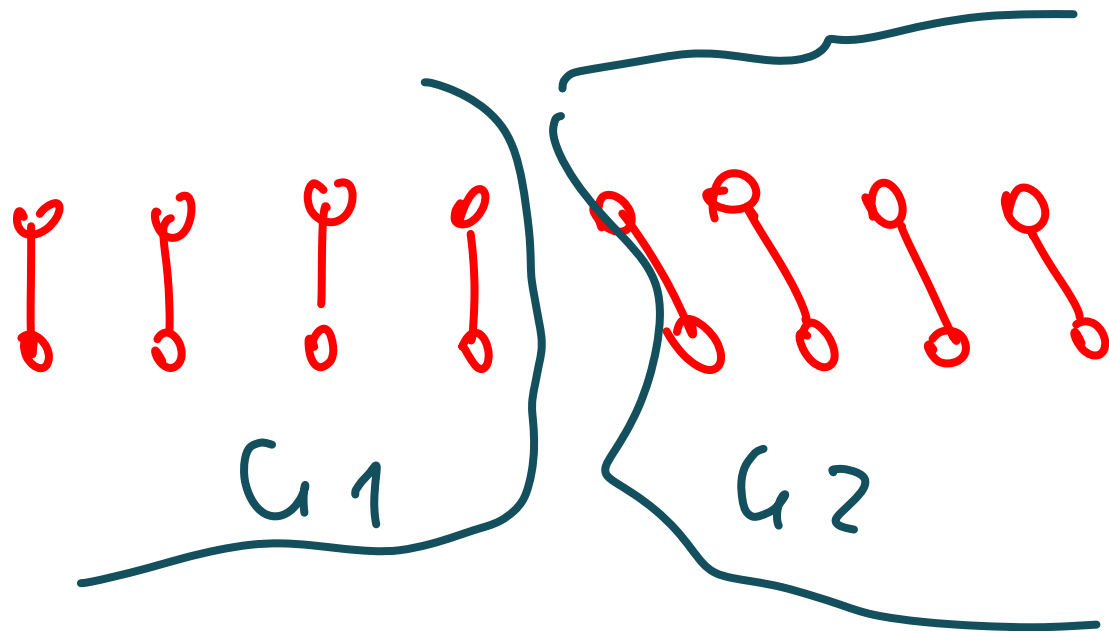


NOT REGULAR

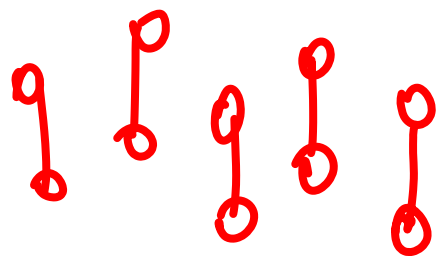
GUIDING WIRE CRYSTAL STRUCTURE - PARAMETERS



- DIFFERENT H. WITHIN EACH GRAIN (INTRA GRAIN)
- (VERTICAL DISPLACEMENT OF WIRE) • ALONG GRAINS (INTER GRAINS)

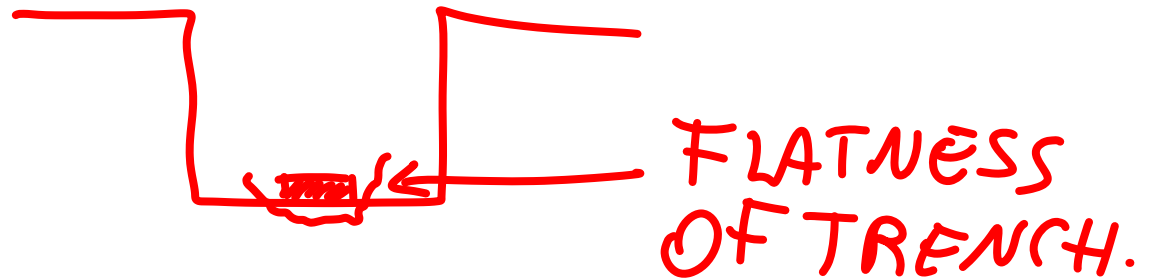


TILT DUE TO
GRAIN
ORIENTATION



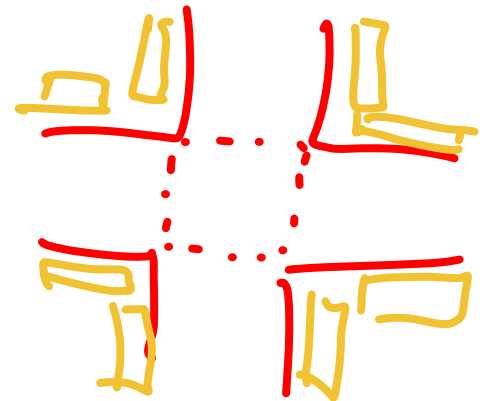
SHIFT DUE TO ANCHORING
POINTS NOT IDEAL

- TRENCH PARAMETERS . H_T , W_T



- ELECTRODE PARAMETERS - DISTANCE BW - ELECTRON.

↳ 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

