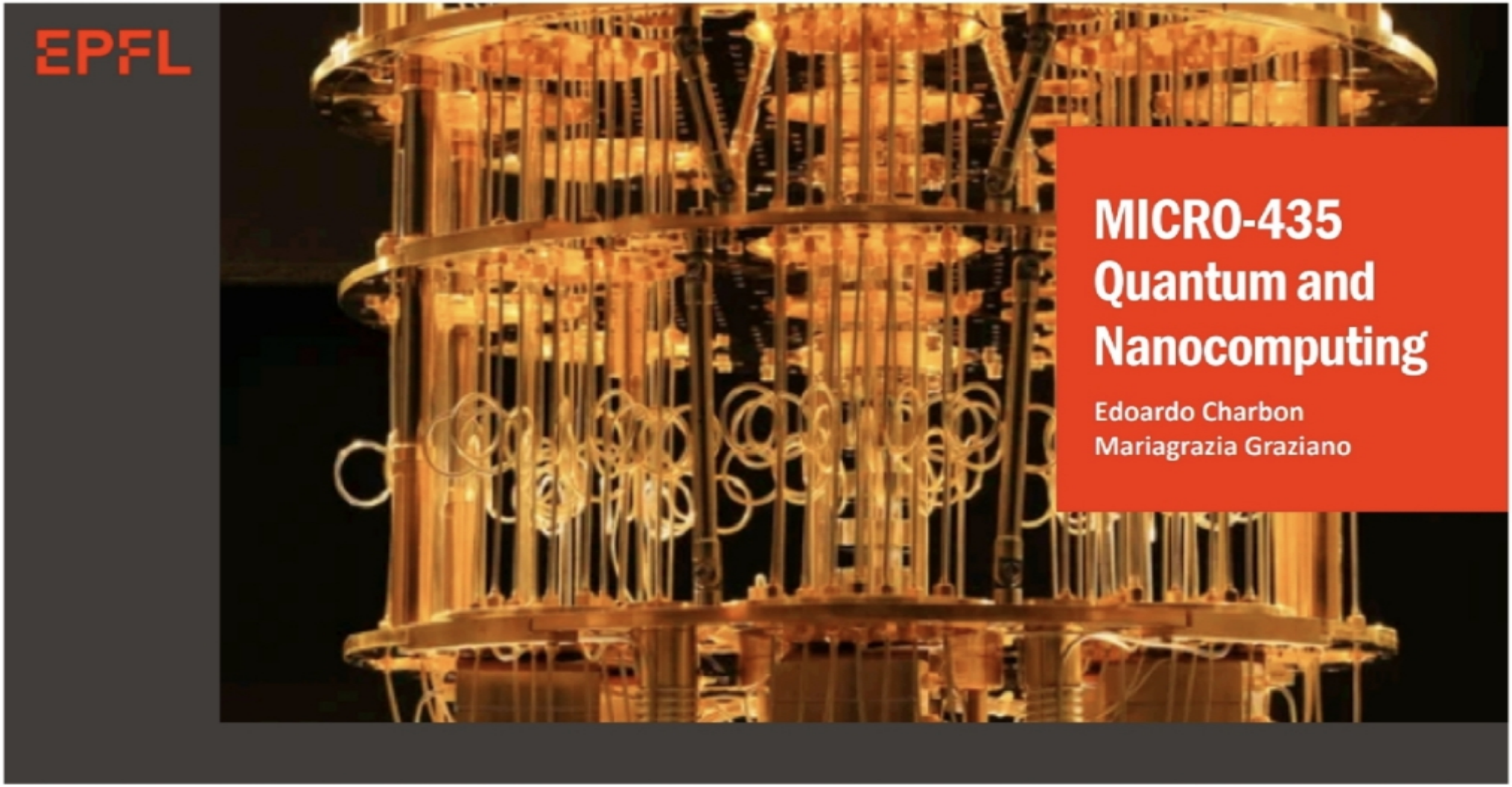


HT FOR MEMORY & SENSORS

OPTIONAL

CIRCUITS BASED ON

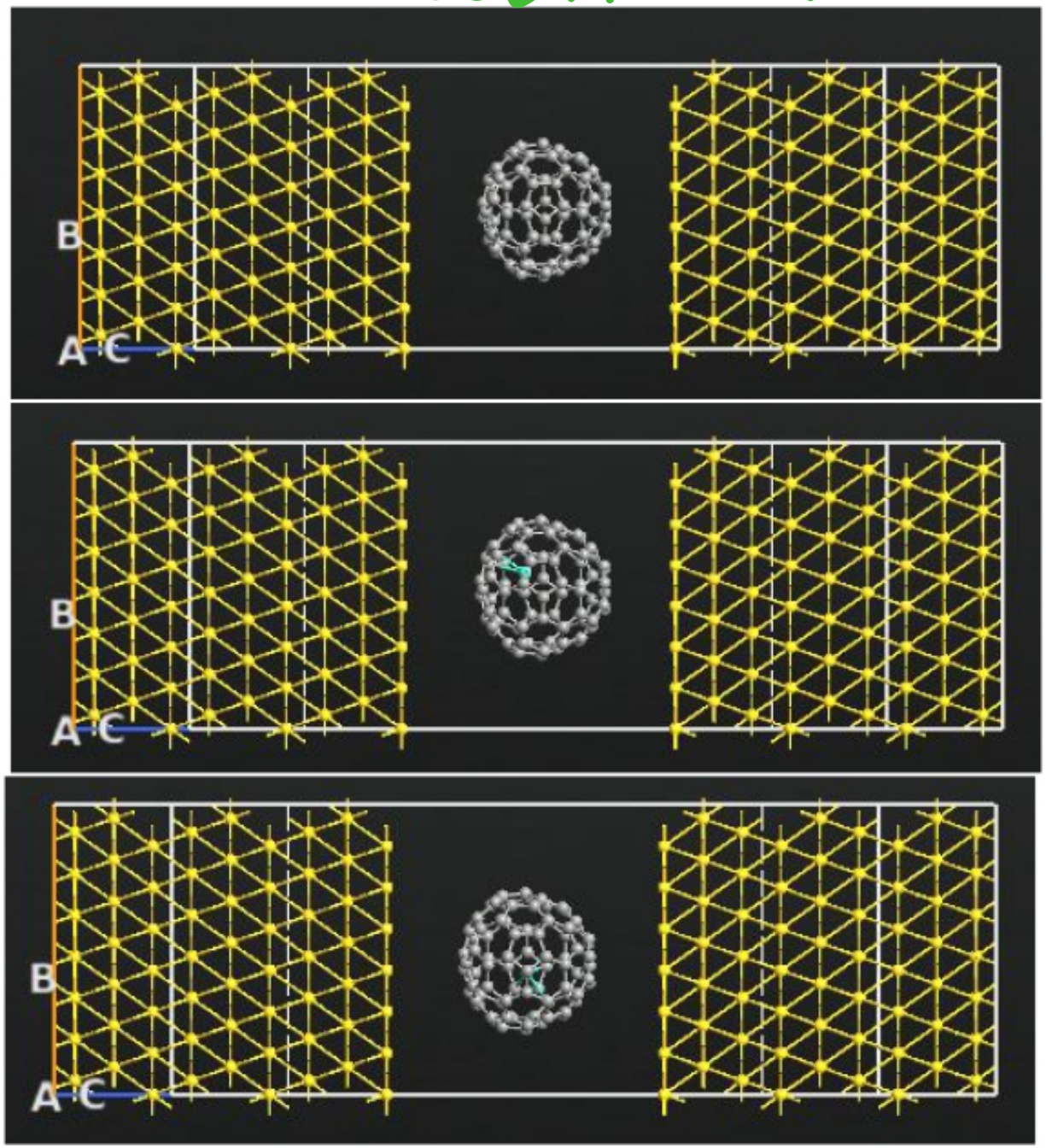
A COUPLE OF OTHER APPLICATIONS

c) ELECTRECT → FERROELECTRY

d) M.T. SENSORS

JUST A QUICK VIEW
MAIN CONCEPTS

ELECTRECT



→ A FULLERENE BESED CAGE C_{82} AND GADOLINIUM TRAPPED INSIDE

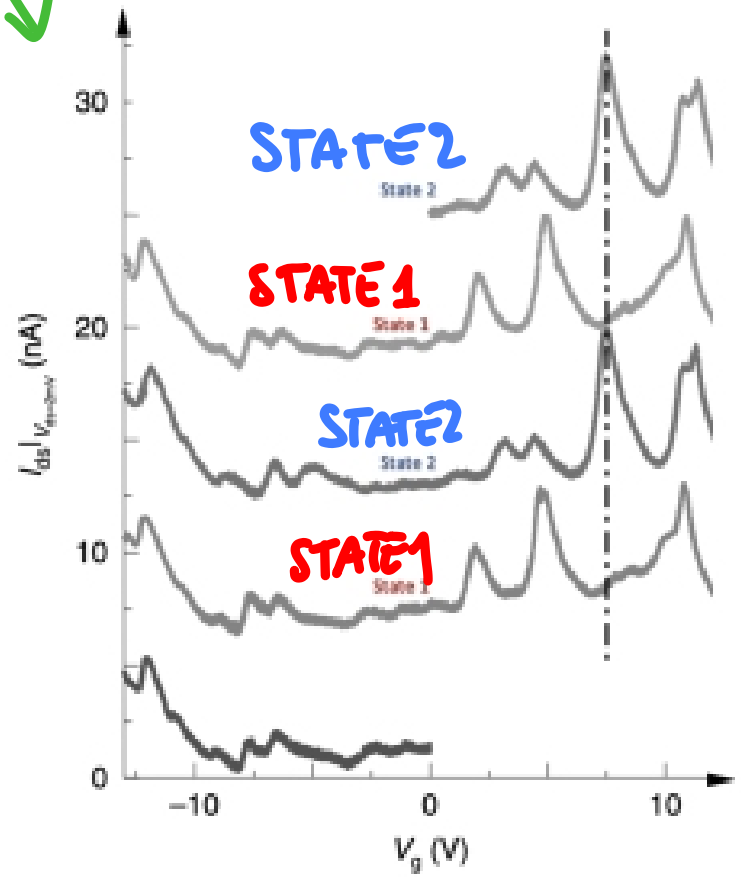
→ ASSUMES 2 STABLE POSITIONS

→ 2 DIFERENT CURRENTS 0 1

MEMORY!!

Gd@C$_{82}$ MOLECULAR TR.

experiment



$I_{DS}(V_G)$ @ $V_{DS} \equiv 2\,mV$

V_G: → INCREASE

DECR. → INCR.

DECR.

TS SHIFTED

BUT WITH HISTERESIS →

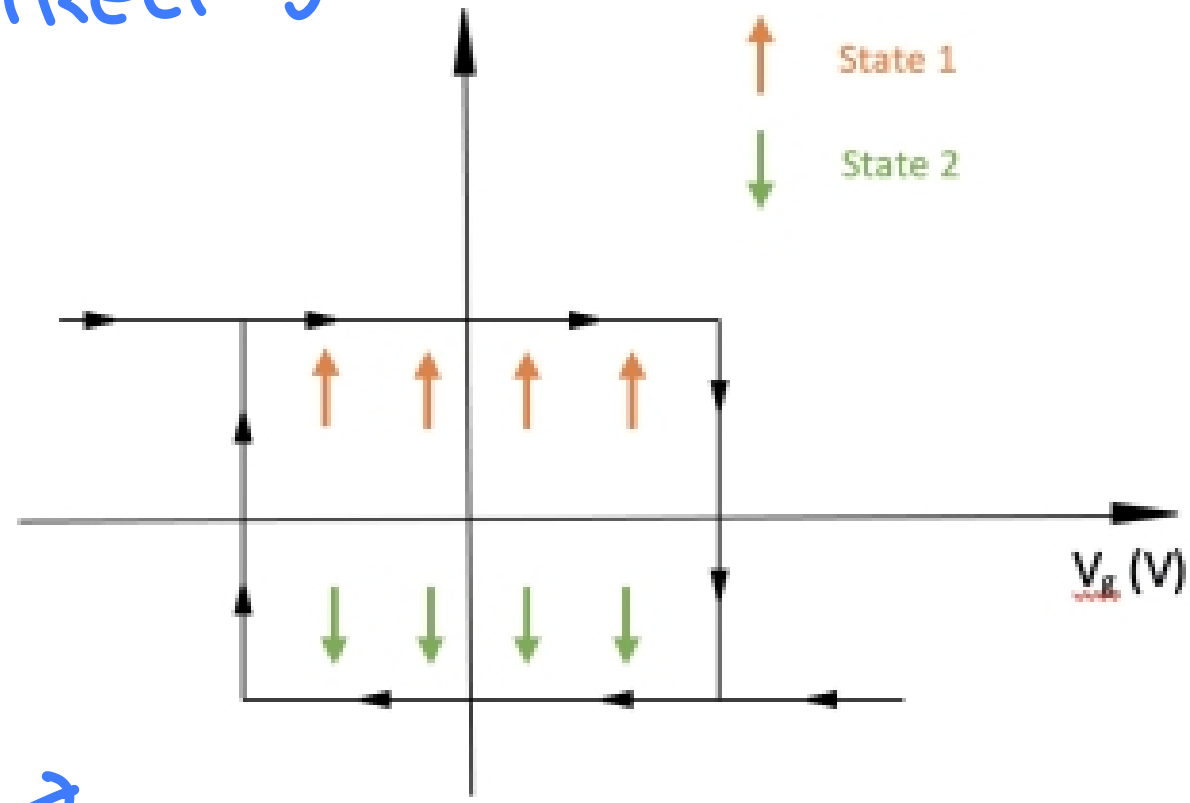
Gd@C$_{82}$ single-mol electrect.

Zhang et. al.

doi: 10.1038/s41565-020-00788-7

GdO C_{82} nT

SINGLE MOLECULE ELECTRECT } SME



$V_G = 0V \Rightarrow$ STATE 1

IT DOES NOT CHANGE EVEN WITH $V_G = -10V$

$V_G > 0$ ↗

WHEN IT REACHE

10 sV

⟹ STATE 2

↗

BEHAVIOR STABLE AND REPATIBLE AND REPRODUCIBLE

GOES BACK TO STATE 1 FOR LARGE $V_G < 0$

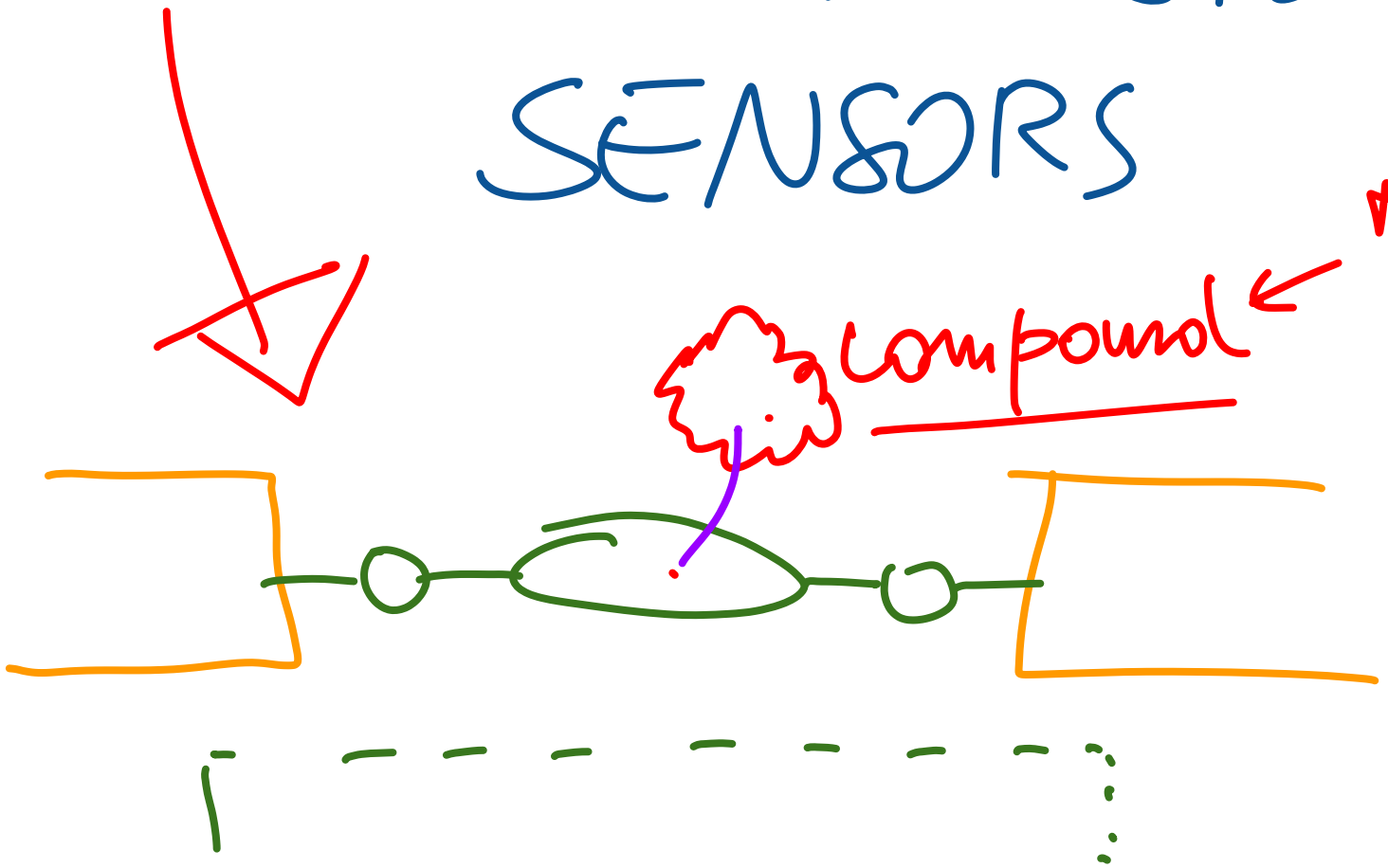
SME

SIMILAR TO FERROELECTRIC MATERIAL

CAN BE USED FOR

SINGLE MOLECULE MEMORY CELL

MOLECULAR TRANSISTOR SENSORS



CASES ANALYZED

CASE ① CYCLOPHANE BASED MOLECULAR SENSOR (CR.)
→ CHEMISORPTION

CASE ② FULLERENE BASED GAS SENSOR
→ PHYSISORPTION

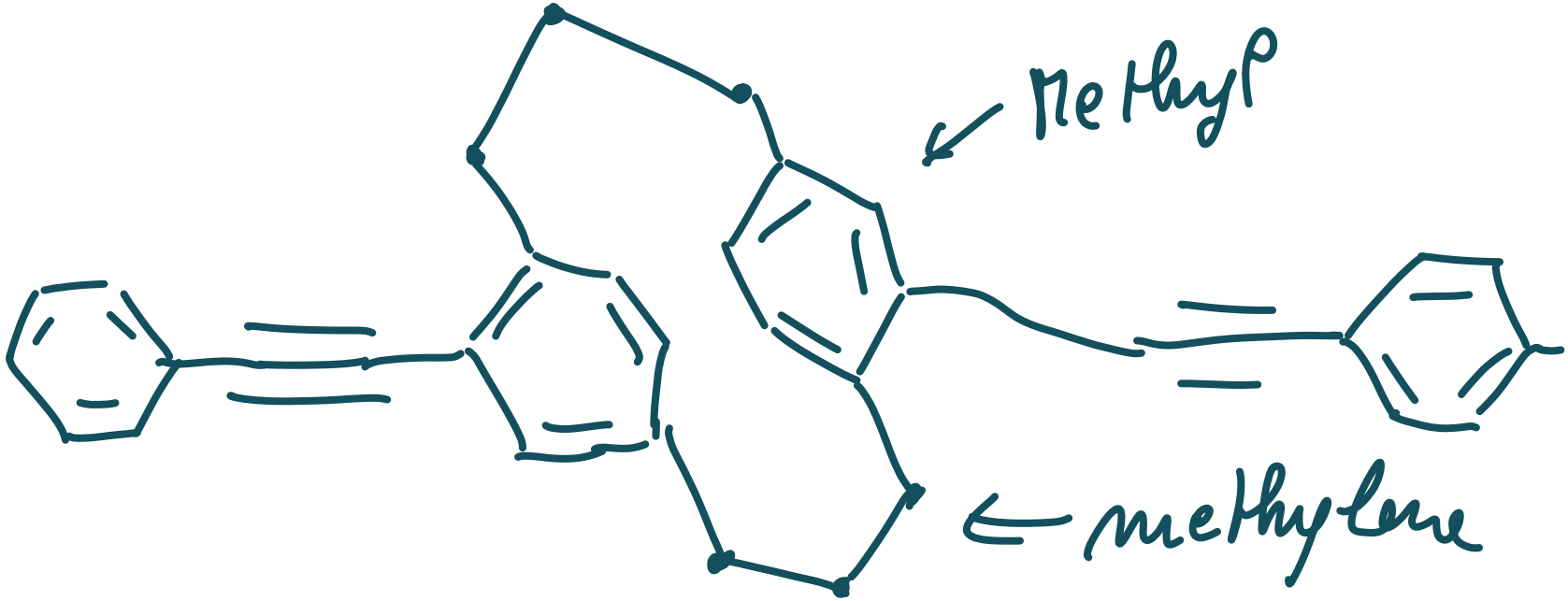
CASE ③ OPE BASE SENSOR FOR THYMINE DETECTION FOR DNA SEQUENCING
→ CHEMISORPTION

CASE 1

CYCLOPHANE-BASED

[3.3]pCp

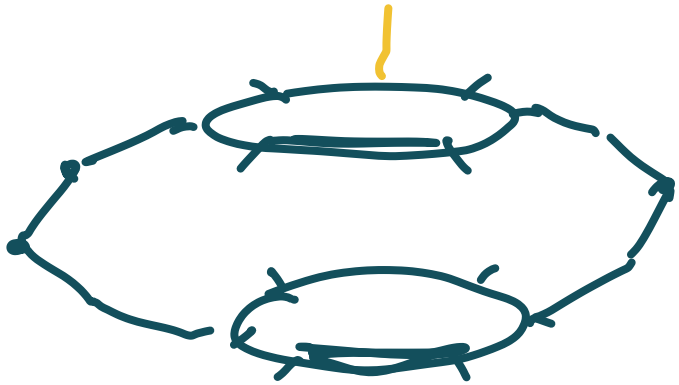
M. SEVS

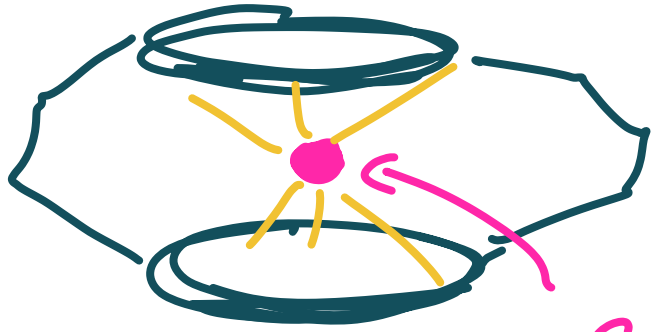


With the whole WIRE

HLG 3.97eV

HLG 2.88eV



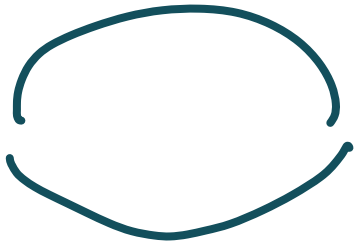


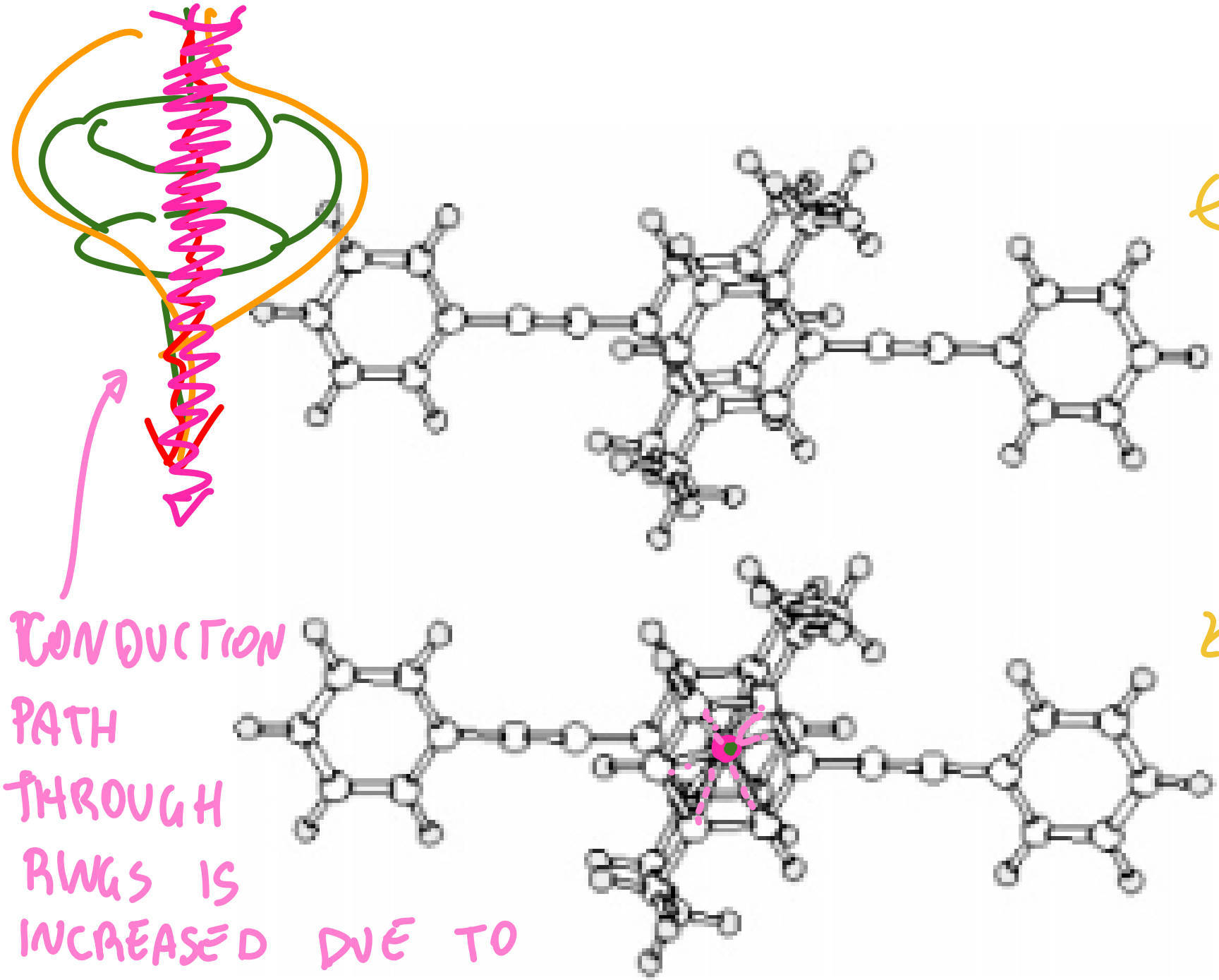
CR

HLG 5.12eV

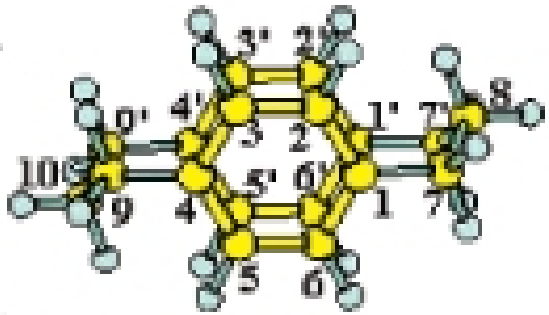
W. CR. → STABILITY INCREASE

HLG 3.84

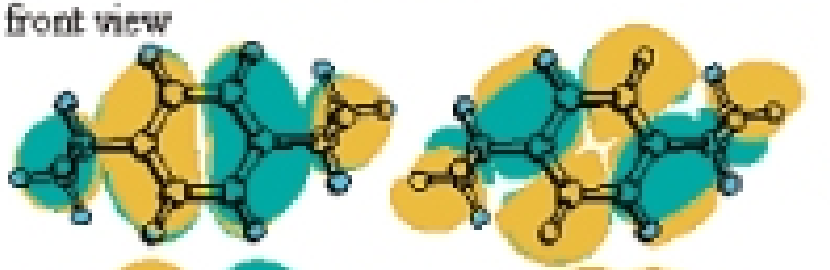



W/o
CR
W
CR
CONDUCTION
PATH
THROUGH
RINGS IS
INCREASED DUE TO
THE METAL PRESENCE

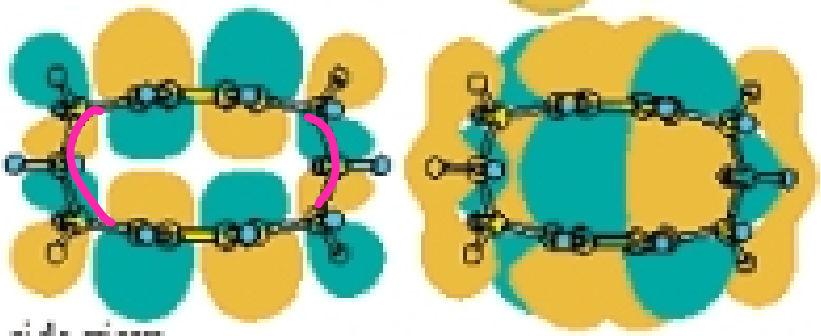
anti



front view



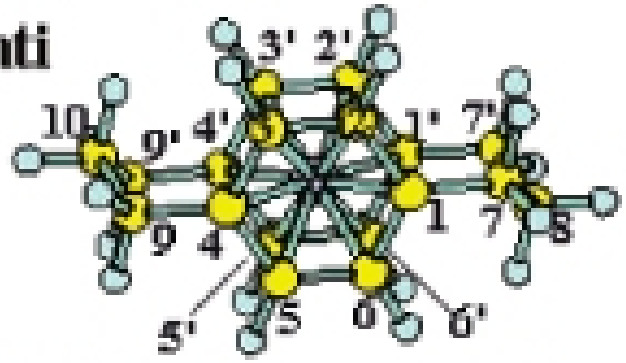
side view



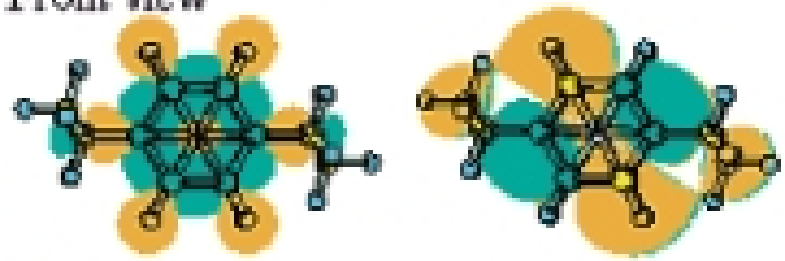
HOMO
-5.73 eV

LUMO
-0.61 eV

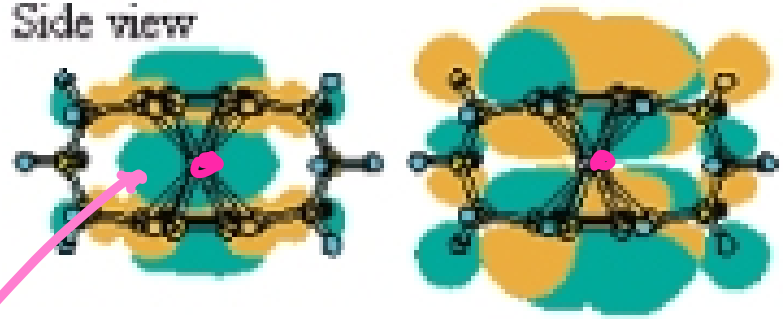
anti



Front view



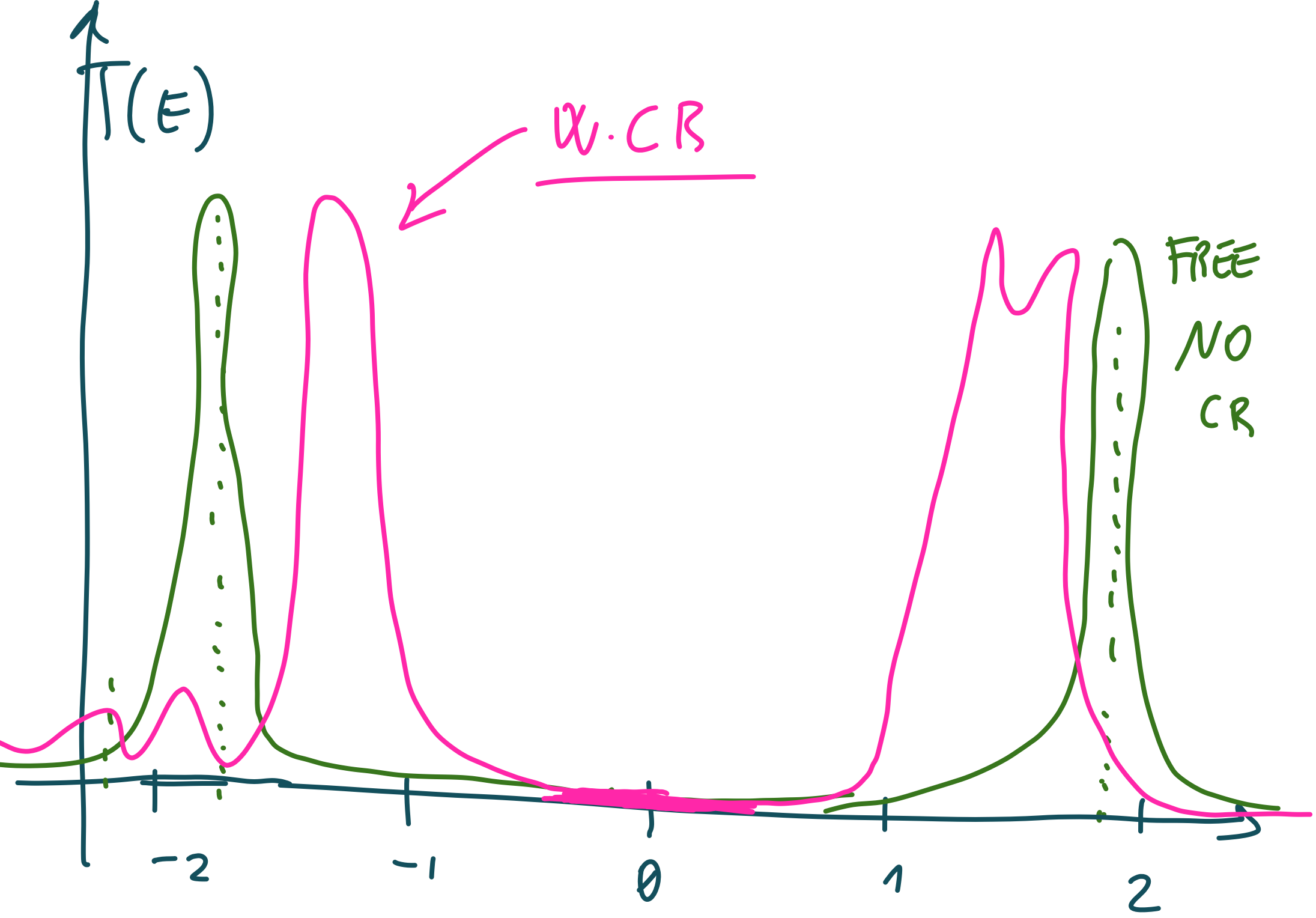
Side view

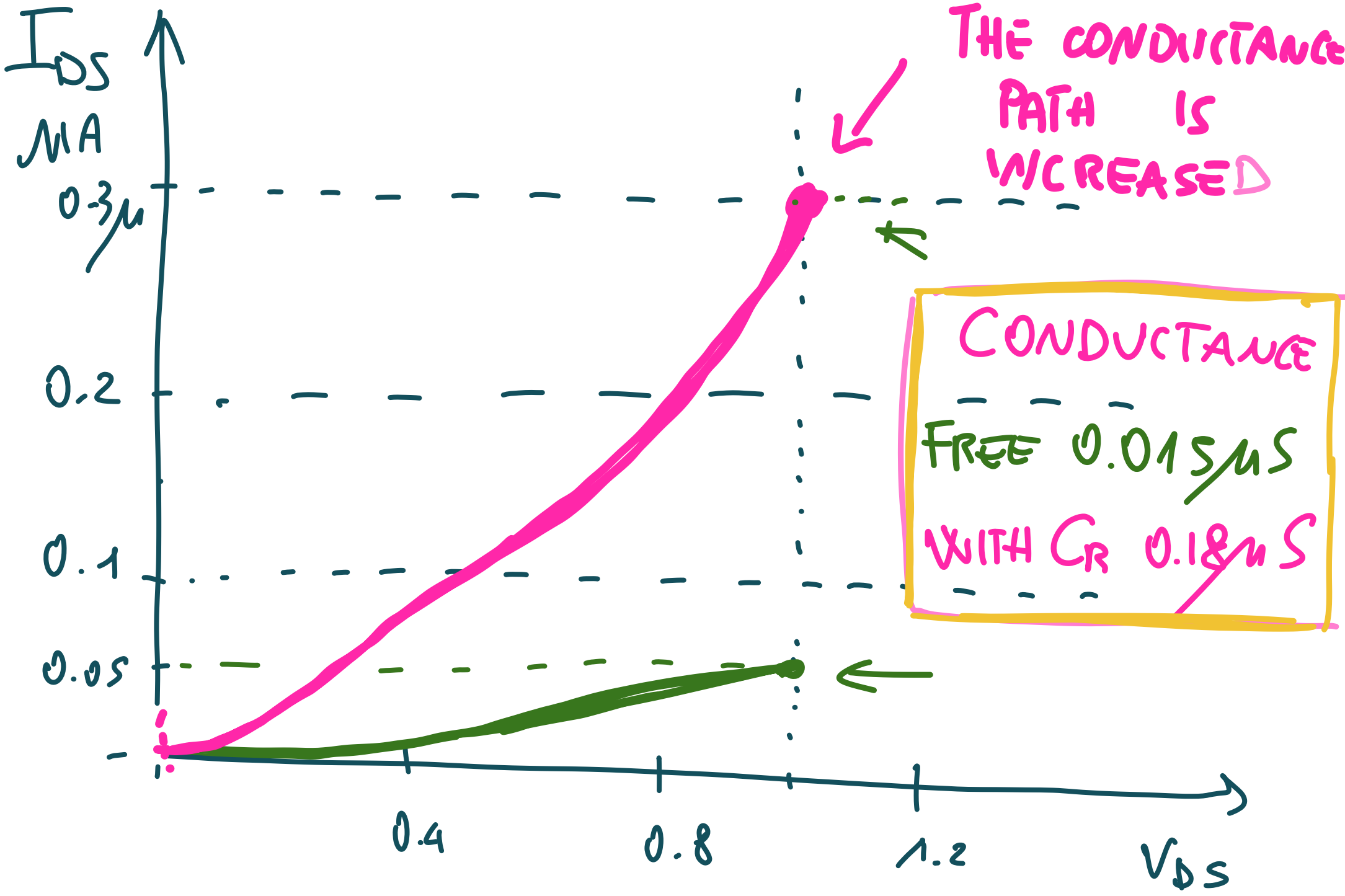


CR SHARES 6 eℓ, 2x6 SHARED BY PHENYL RINGS

HOMO
-4.08 eV

LUMO
-0.24 eV


T(E)
W. CR
FREE
NO
CR
-2
-1
0
1
2

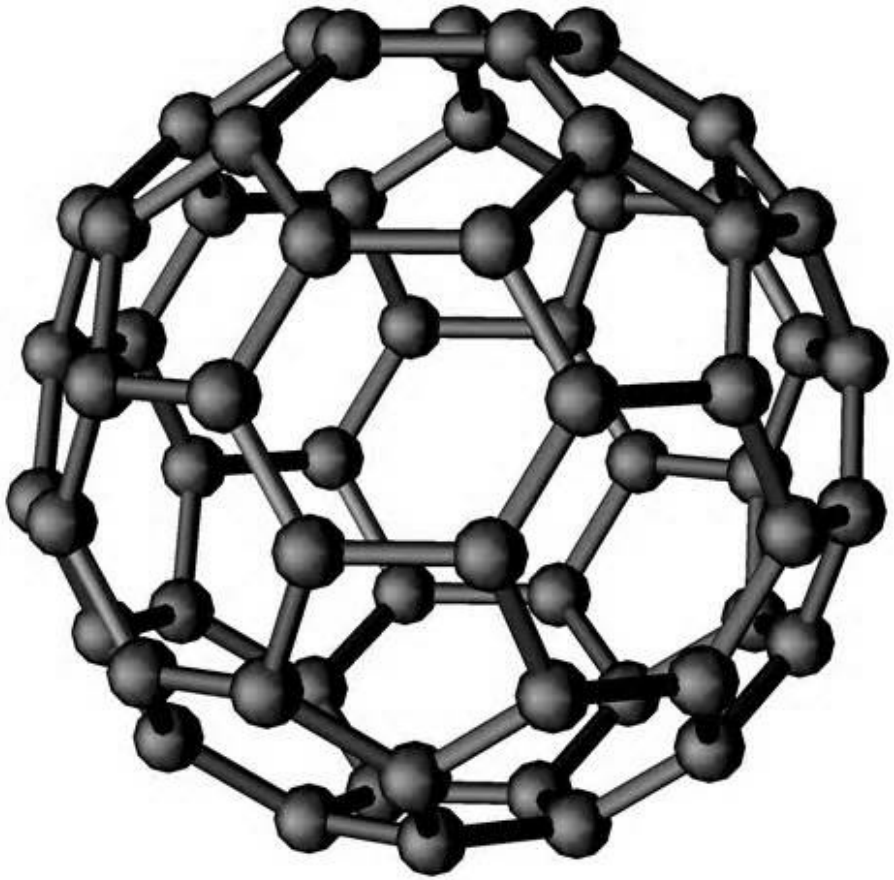

I_{DS}
MA
0.3μ
0.2
0.1
0.05
0.4
0.8
1.2
V_{DS}
THE CONDUCTANCE PATH IS INCREASED
CONDUCTANCE
FREE 0.015μS
WITH C_R 0.18μS

CASE 2

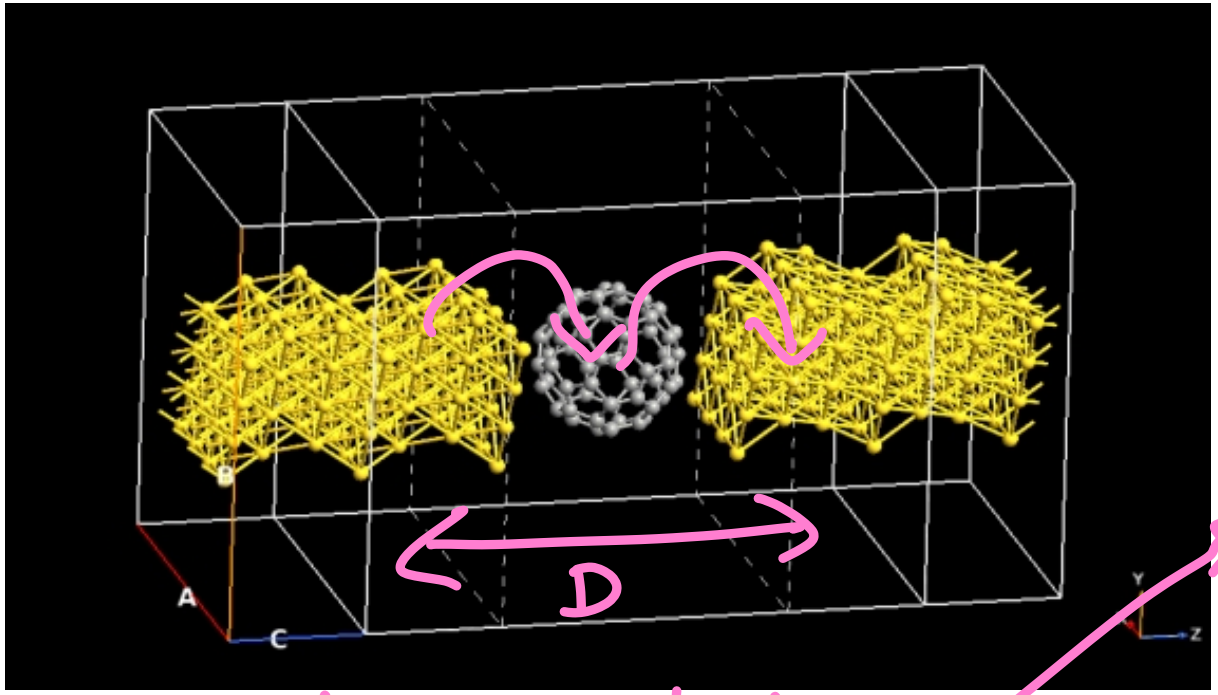
GAS SENSOR BASED ON FULLERENE

$2(10+N)$ CARBON ATOMS

C_{60}



$d \approx 7\text{Å}$

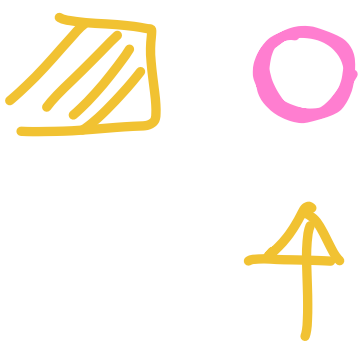


depending on distance → weak coupling

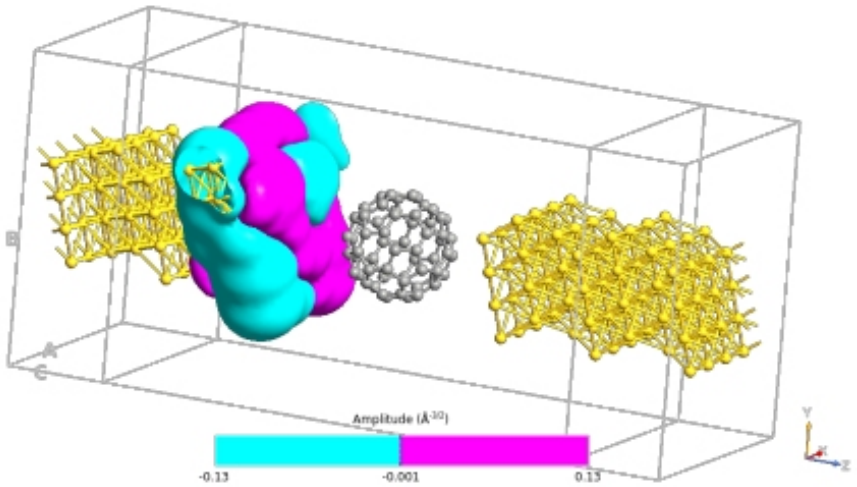
→ strong coupling

CASE STUDY

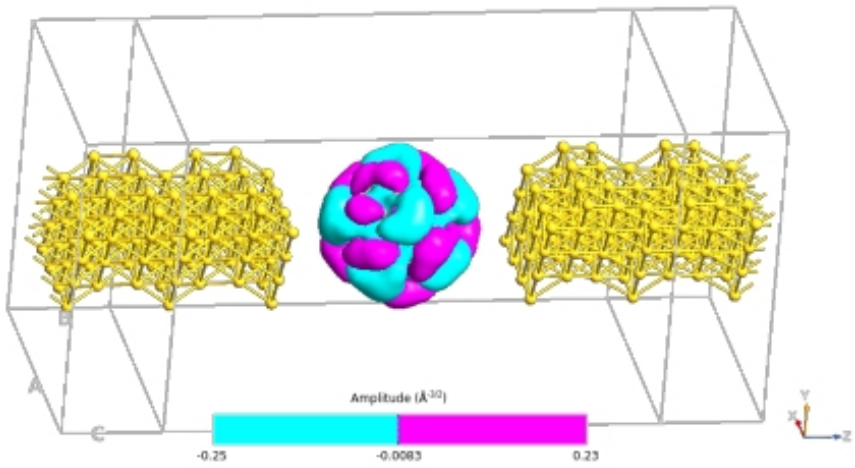
GOLD



Pt

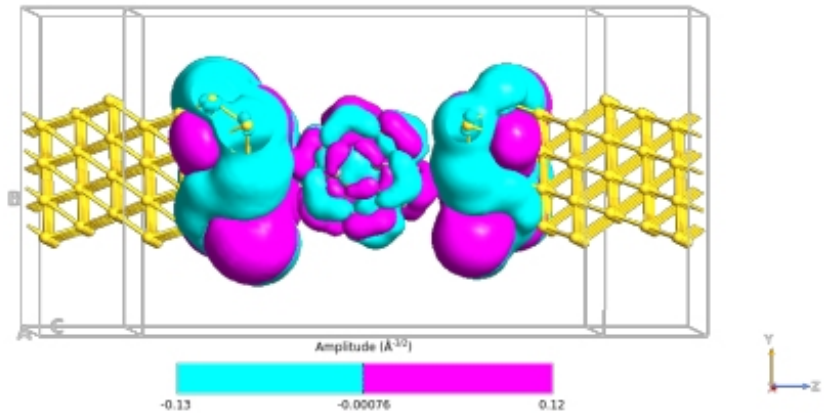


(a) HOSO 3A

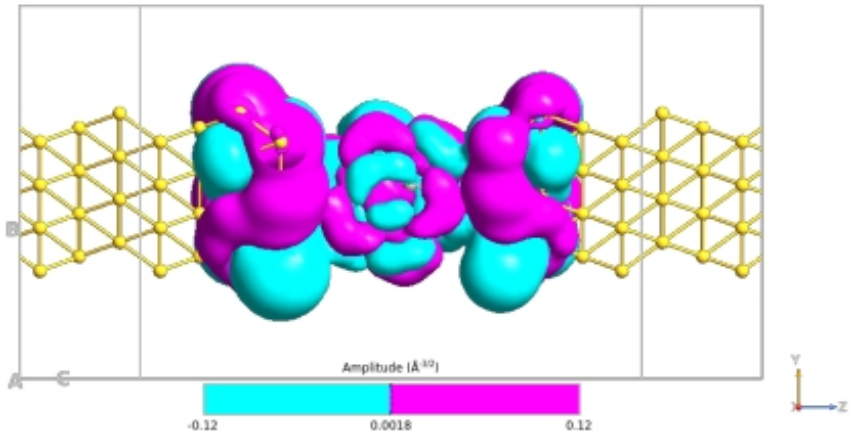


(b) LUSO

igure 8.11: MPSH of the HOSO (Highest Occupied System Orbital) and the LUSO (Lowest Unoccupied System Orbital) of the C_{60} molecular wire with molecule-contact distances of 5.4 Å. The two colors (teal and fuchsia) are referred to the phase (negative or positive) of the MPSH. The figure was generated by *ATK* software [**ATK2020**], [**ATK_vQ2019d12**] (used for performing the simulations).

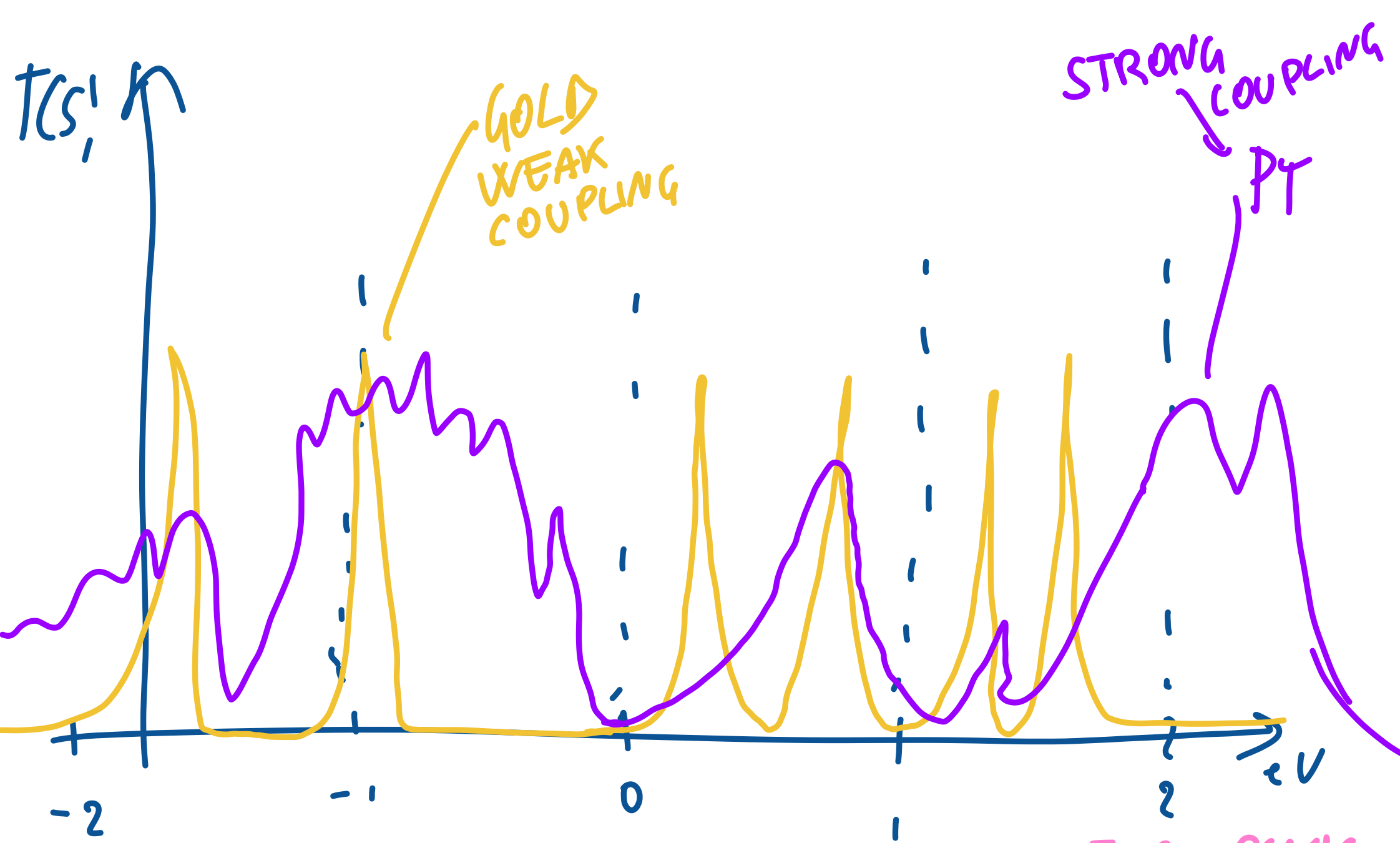


(a) 4 Å 4A

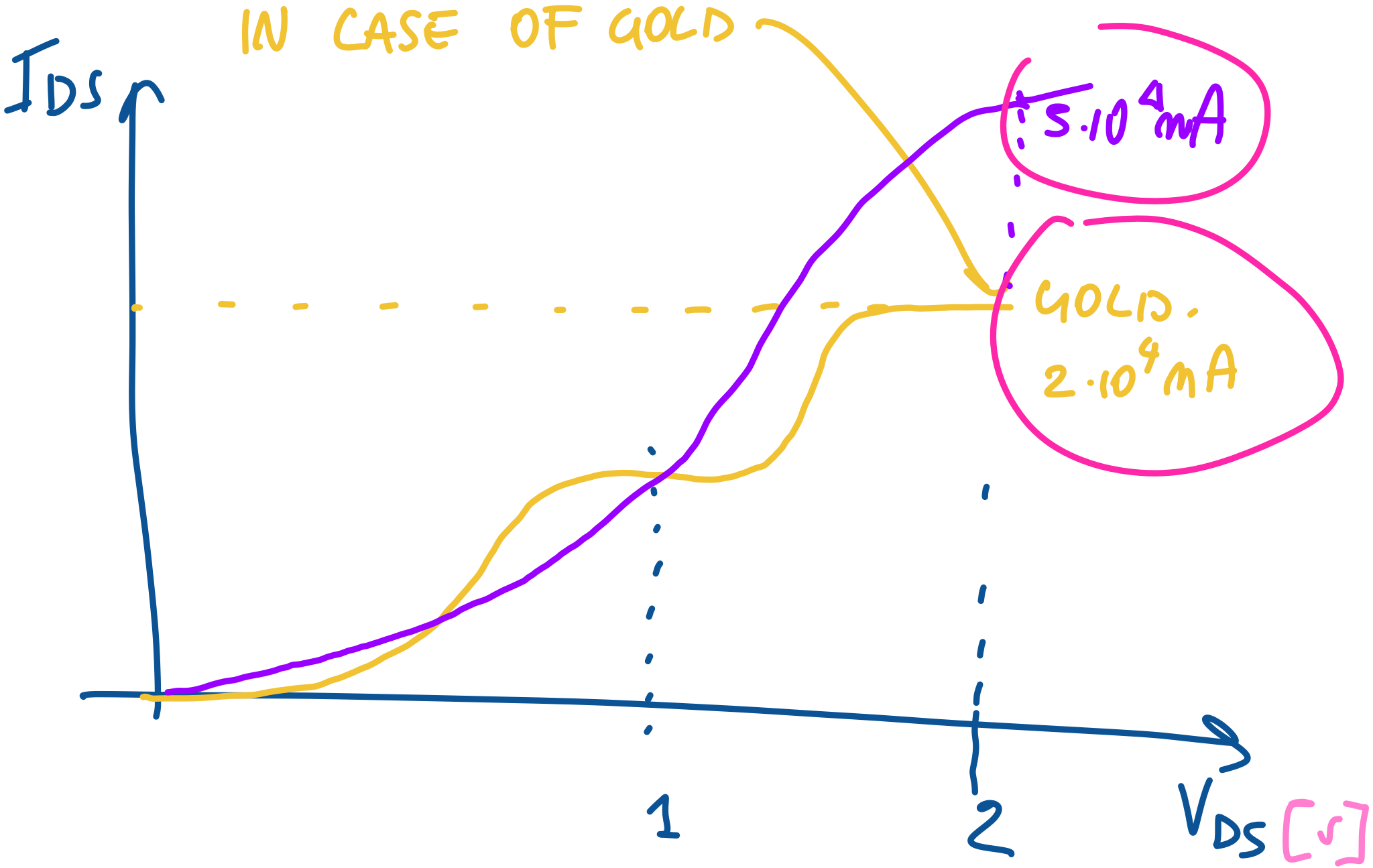


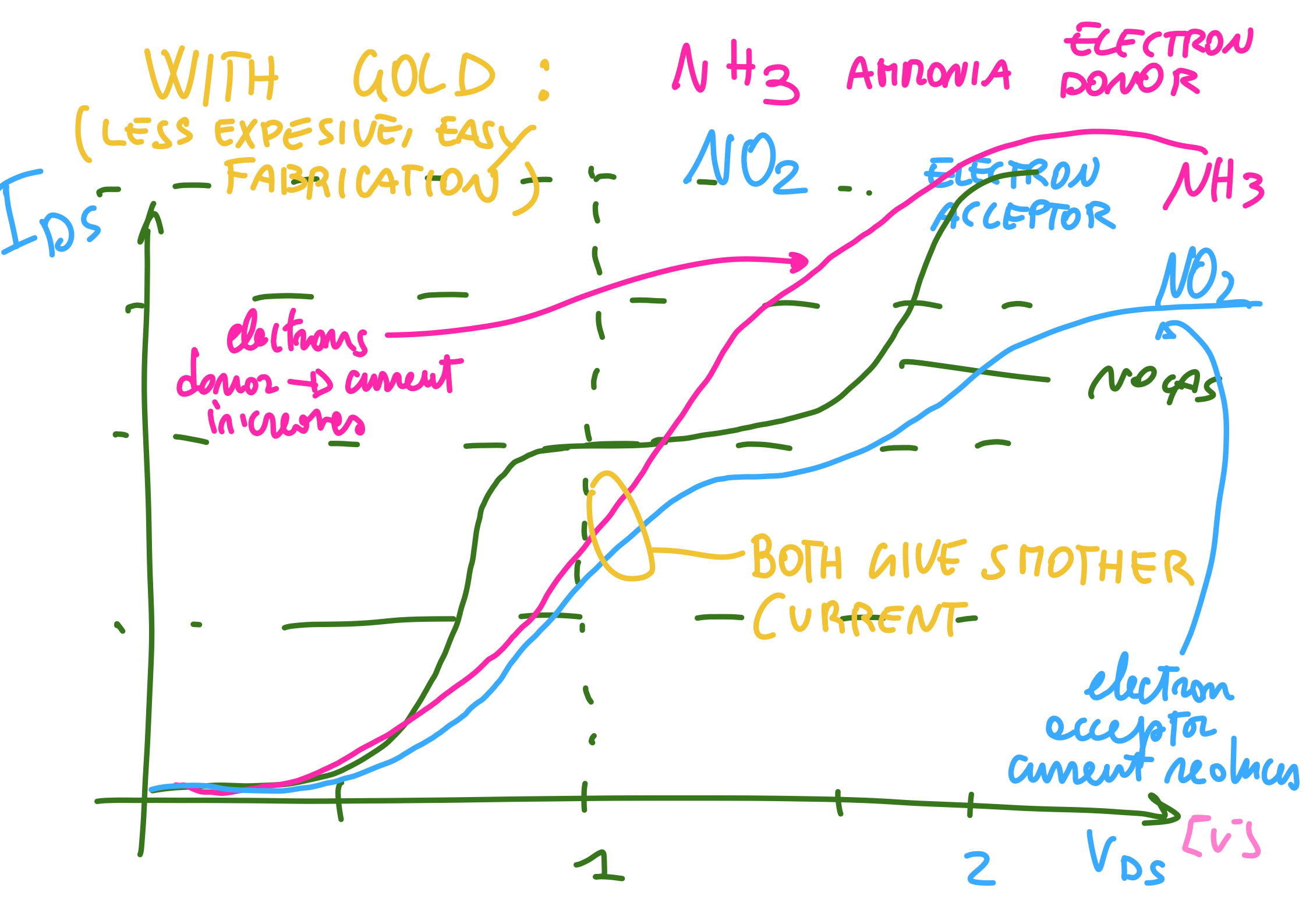
(b) 3 Å 3A

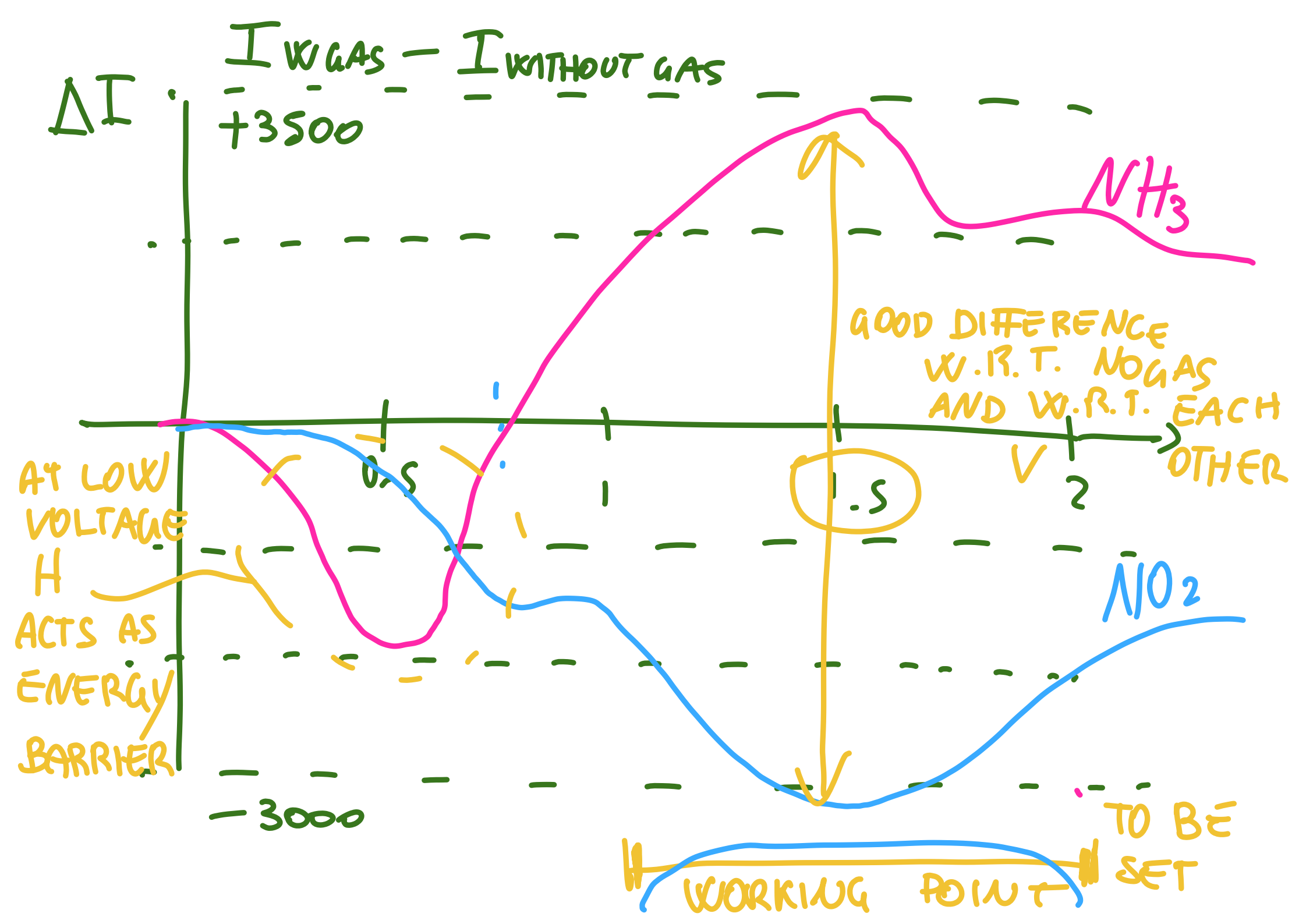
Figure 8.12: MPSH of the HOSO (Highest Occupied System Orbital) of the C_{60} molecular wire with molecule-contact distances of 4 Å and 3 Å, respectively. The two colors (teal and fuchsia) are referred to the phase (negative or positive) of the MPSH. The figure was generated by *ATK* software [**ATK2020**], [**ATK_vQ2019d12**] (used for performing the simulations).

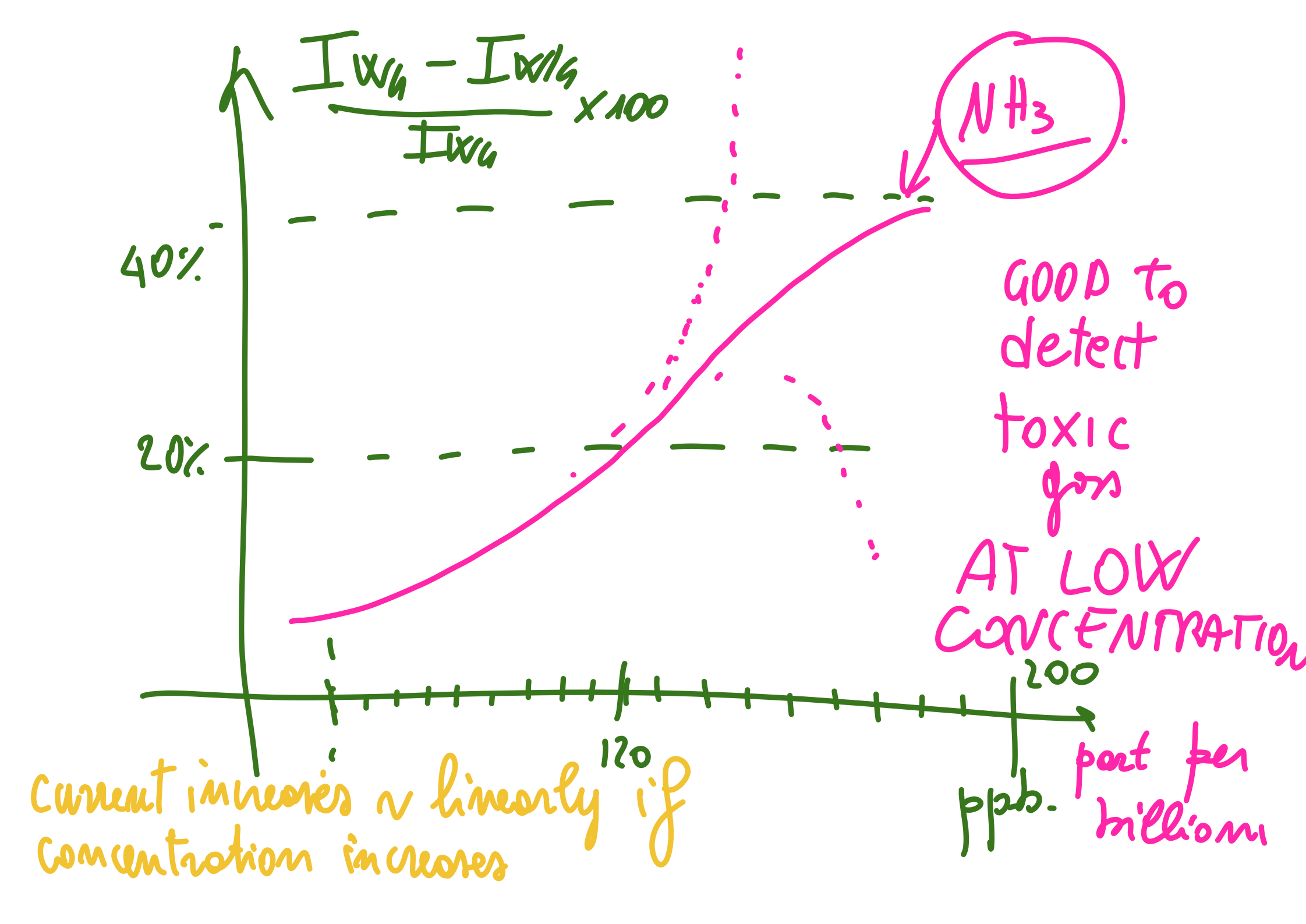


THE CHOICE OF ELECTRODE CAN INFLUENCE THE COUPLING B/W ELECTRODES & MOLECULAR SYSTEM, CAN BE EXPLOITED DEPENDING ON APPLICATION

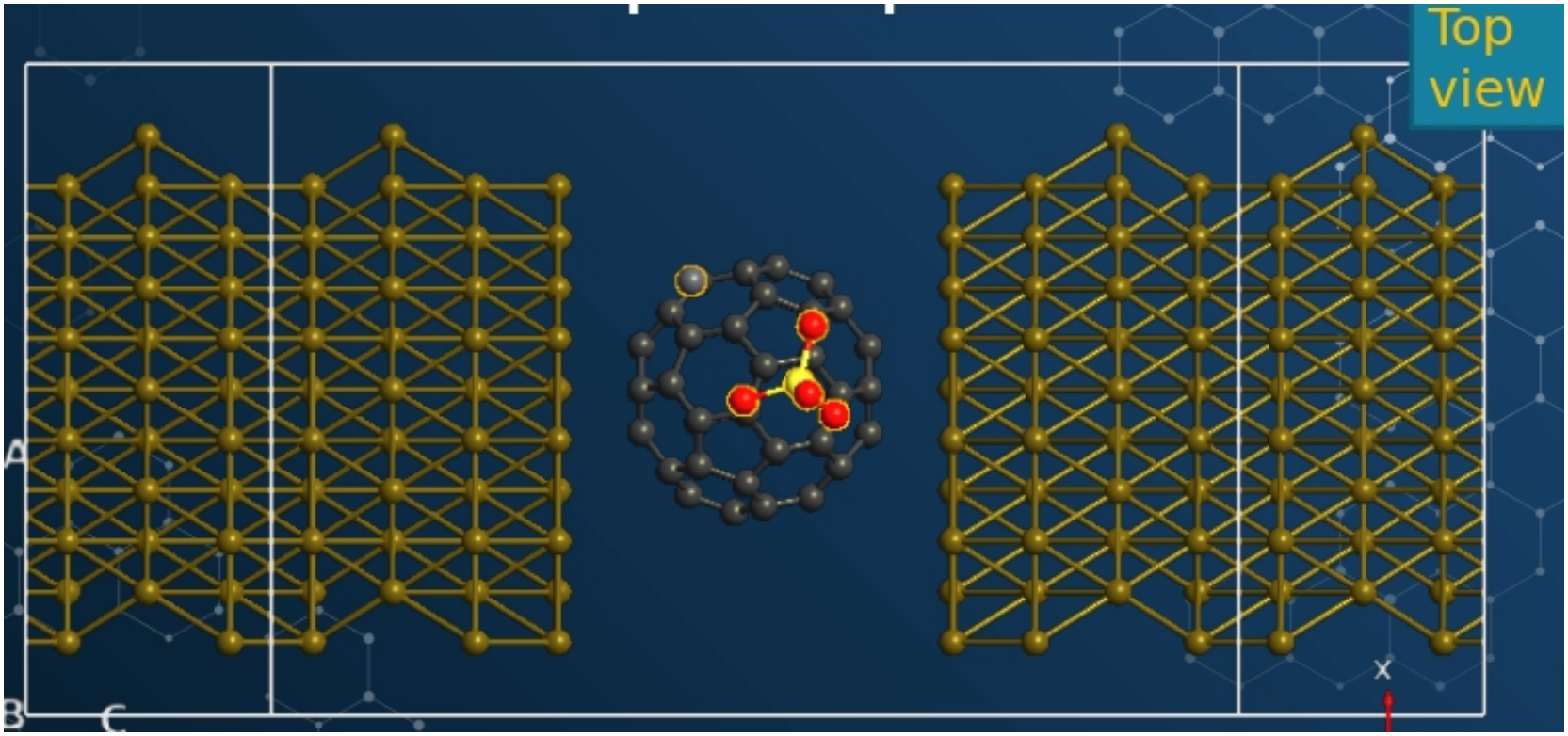

IN CASE OF GOLD
I_{DS}
$5 \cdot 10^{-4}$ mA
GOLD.
$2 \cdot 10^{-4}$ mA
1
2
V_{DS} [V]


WITH GOLD :
(LESS EXPESIVE, EASY FABRICATION)
NH_3 AMMONIA
ELECTRON DONOR
NO_2
ELECTRON ACCEPTOR
I_{DS}
NH_3
NO_2
electrons donor → current increases
NO GAS
BOTH GIVE SMOTHER CURRENT
electron acceptor current reduces
1
2
V_{DS} [V]

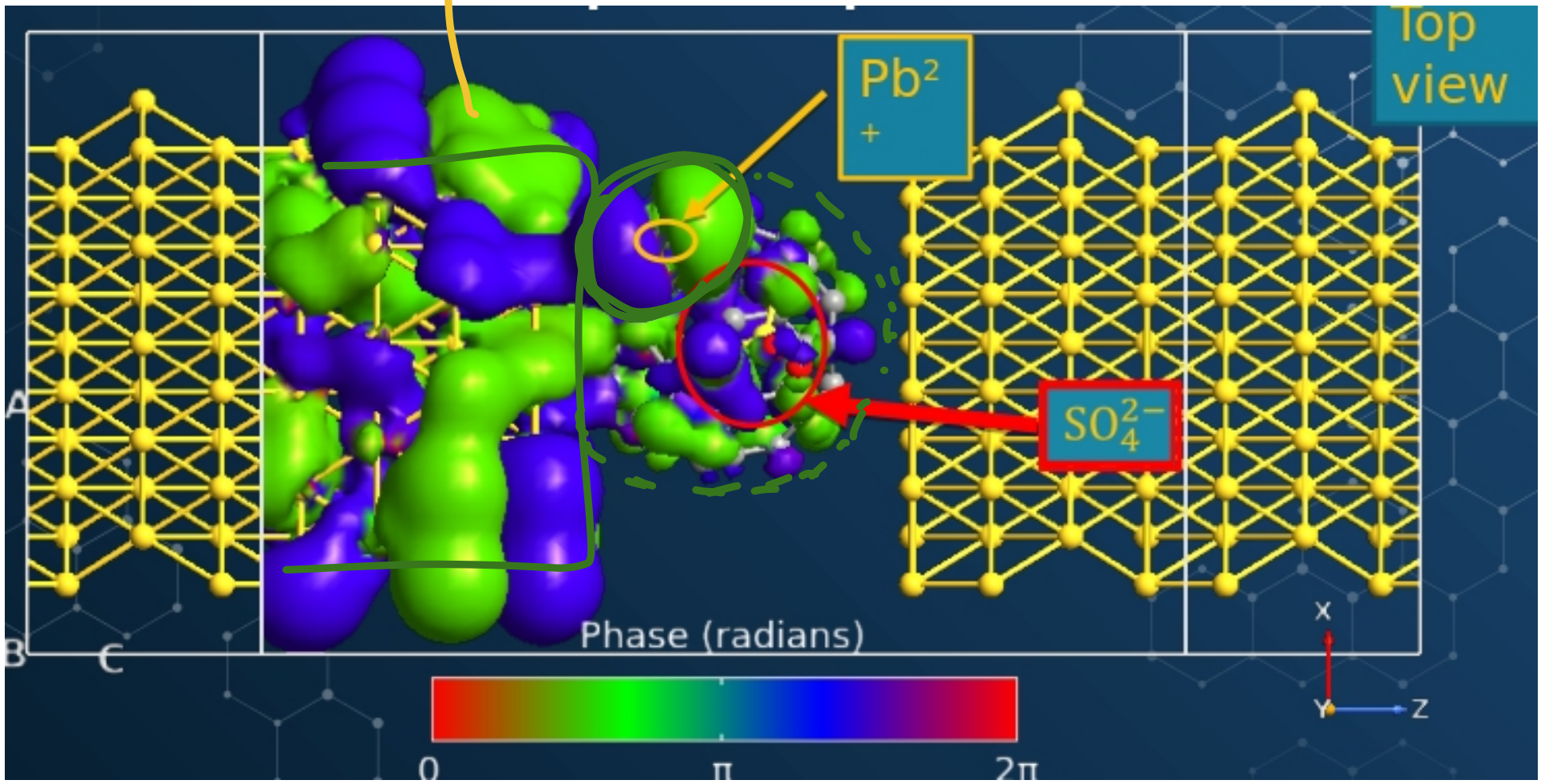

$I_{WGAS} - I_{WITHOUT\ GAS}$
ΔI
+3500
−3000
0.5
1
1.5
2
V
NH_3
NO_2
GOOD DIFFERENCE W.R.T. NOGAS AND W.R.T. EACH OTHER
AT LOW VOLTAGE H ACTS AS ENERGY BARRIER
WORKING POINT
TO BE SET

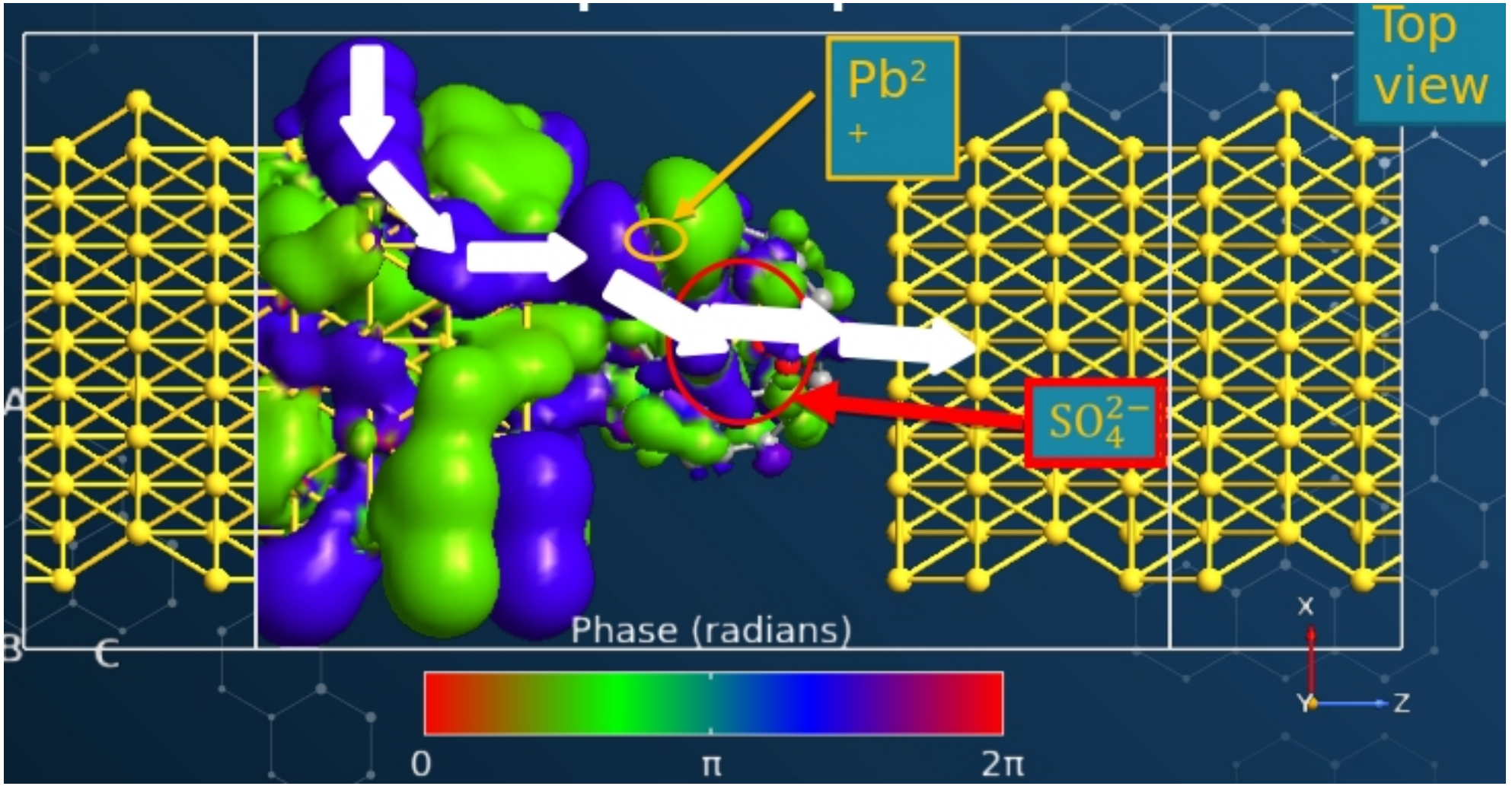

$\frac{I_{WG} - I_{WOG}}{I_{WG}} \times 100$
40%
20%
NH_3
GOOD to detect toxic gas AT LOW CONCENTRATION
120
200
ppb.
part per billion
Current increases linearly if concentration increases

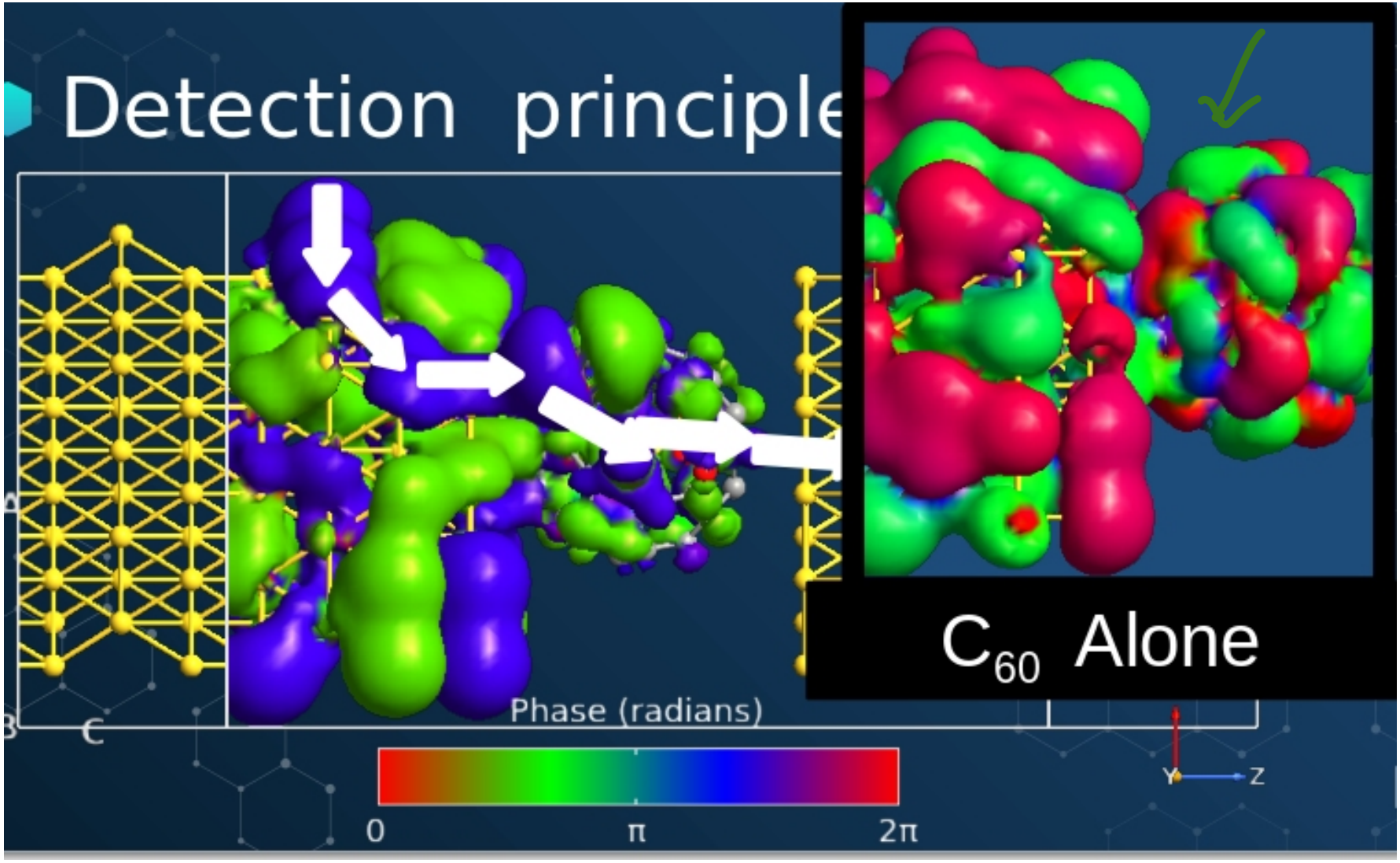
GAS SENSOR : $PbSO_4$ WITH FULLERENE

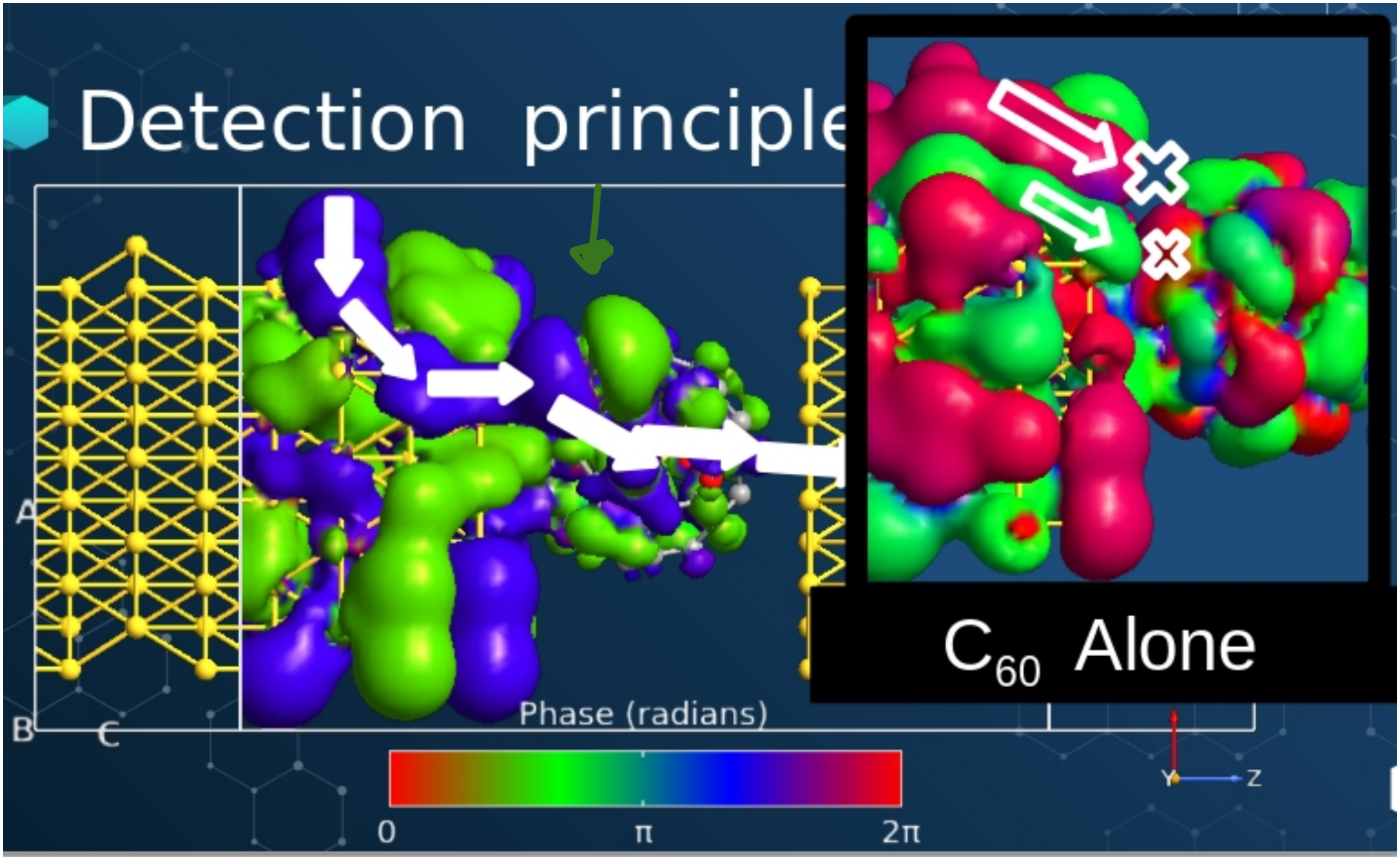


REGION OF SPACE WHERE TRANSMISSION OCCURS - ISOSURFACES OF TRANSMISSION




Top view
Pb²⁺
SO_4^{2-}
Phase (radians)
0
π
2π
X
Y
Z
A
B
C


Detection principle
Phase (radians)
0
π
2π
C_{60} Alone
Y
Z


Detection principle
A
B
C
Phase (radians)
0
π
2π
Y
Z
C60 Alone

CASE 3 MOLECULAR SENSOR FOR DETECTION OF THYMINE IN DNA SEQUENCING

IN DNA 4 NUCLEOBASE

G C A T

GUANINE

THYMINE

ADENINE

CYTOSINE

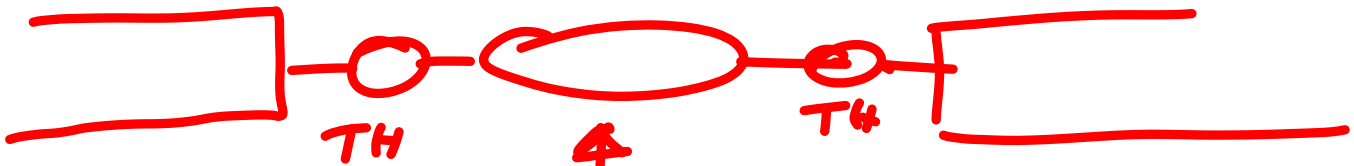
GGCAATGC - - - - - - - - -

LD BLAST

TRANSDUCERS ARE NEEDED → 1 ELEMENT IN DNA

PROCESSING ← IN // ← ELECTRICAL INF

THE SENSOR

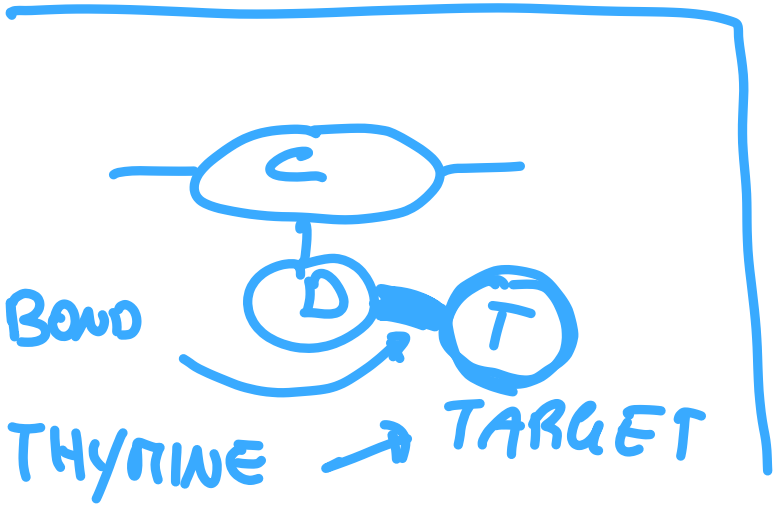


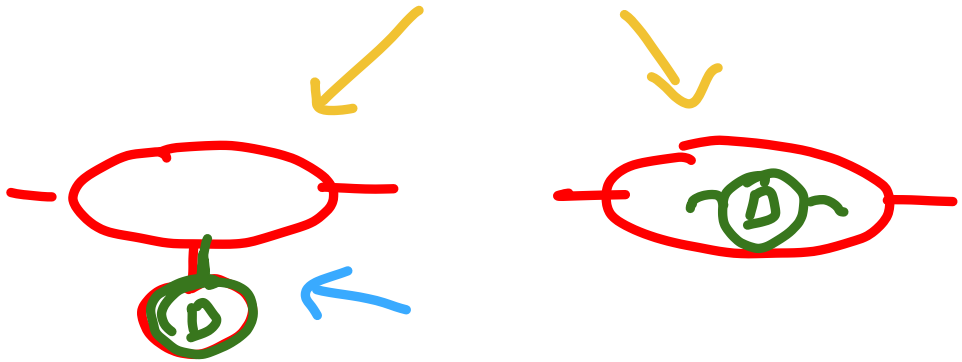
CONDUCTION UNIT

responsible of conduction in channel

DETECTION UNIT

CONNECTED AS

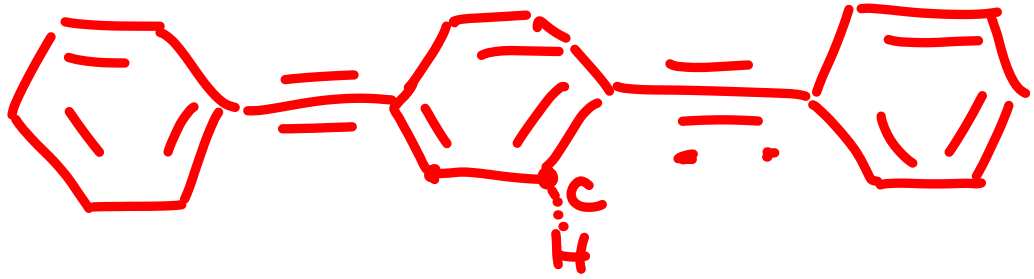




IN THIS CASE

CONDUCTION UNIT

OPE

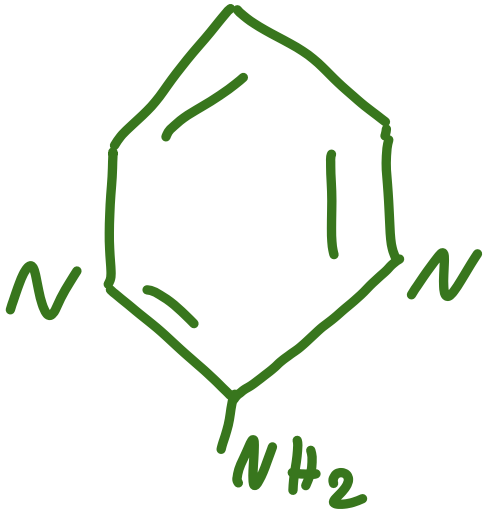


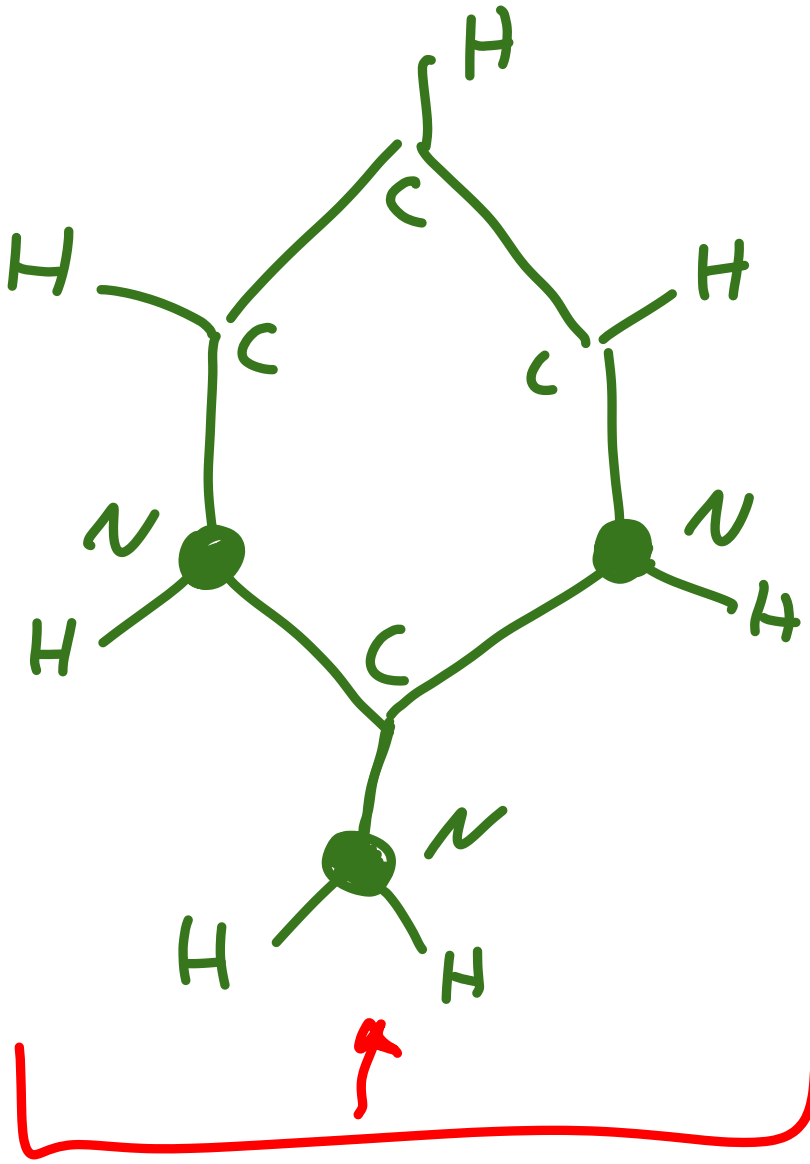
DETECTION UNIT

2-AMIN PYRAMIDINE

PHYRAMIDINE

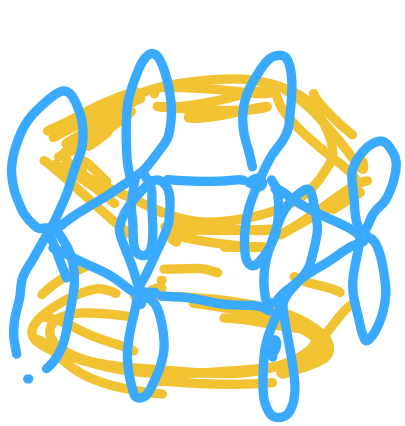
DETECTION UNIT

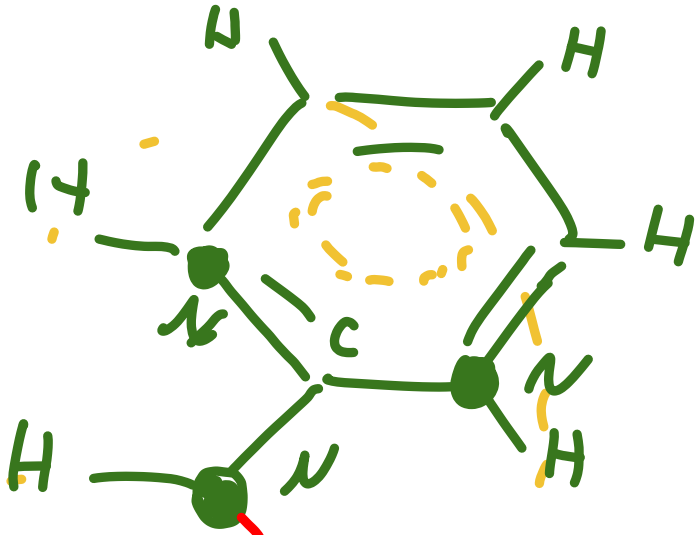




CONNECTED TO
THE CONDUCTION UNIT

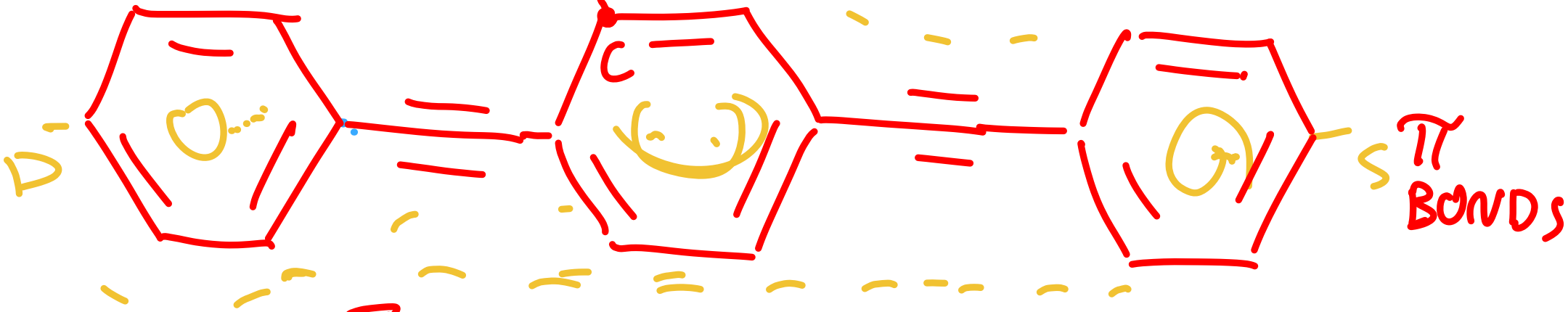
SENSOR MOLECULE CONDUCTIVE + DECTION





DET

π BONDS



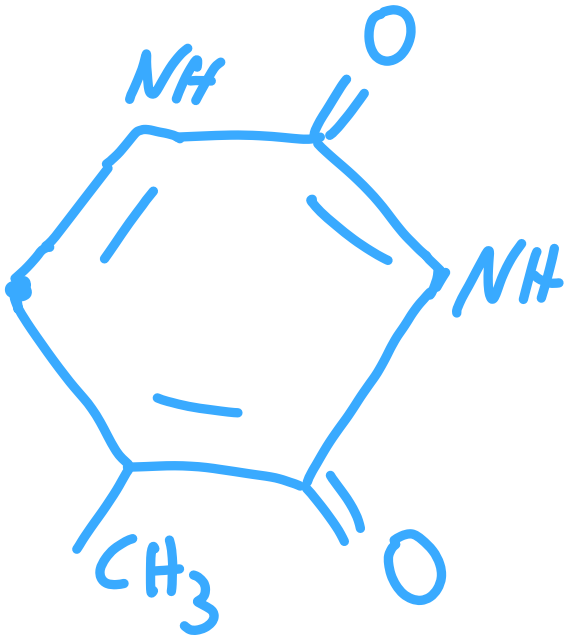
π BONDS

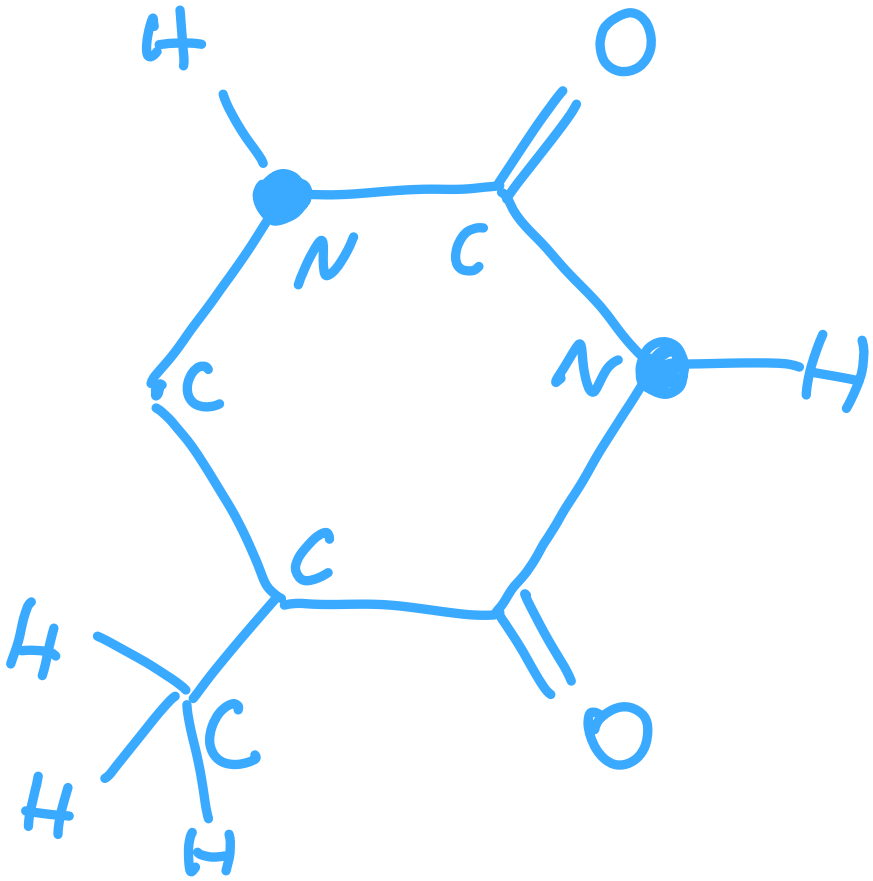
PLANAR STRUCTURE

CONJUGATED SYSTEM

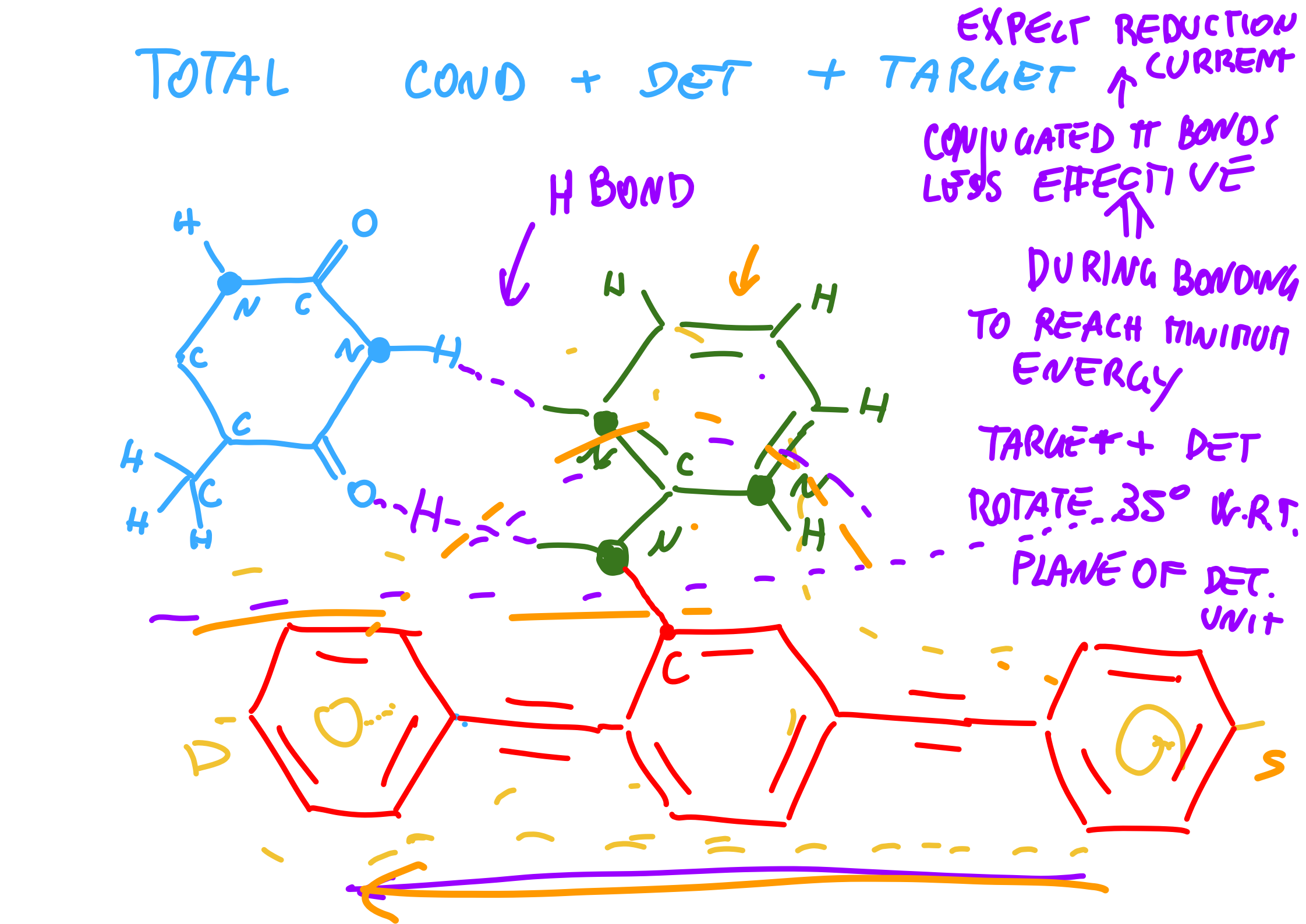
TARGET THYMINE $C_5H_6N_2O_2$

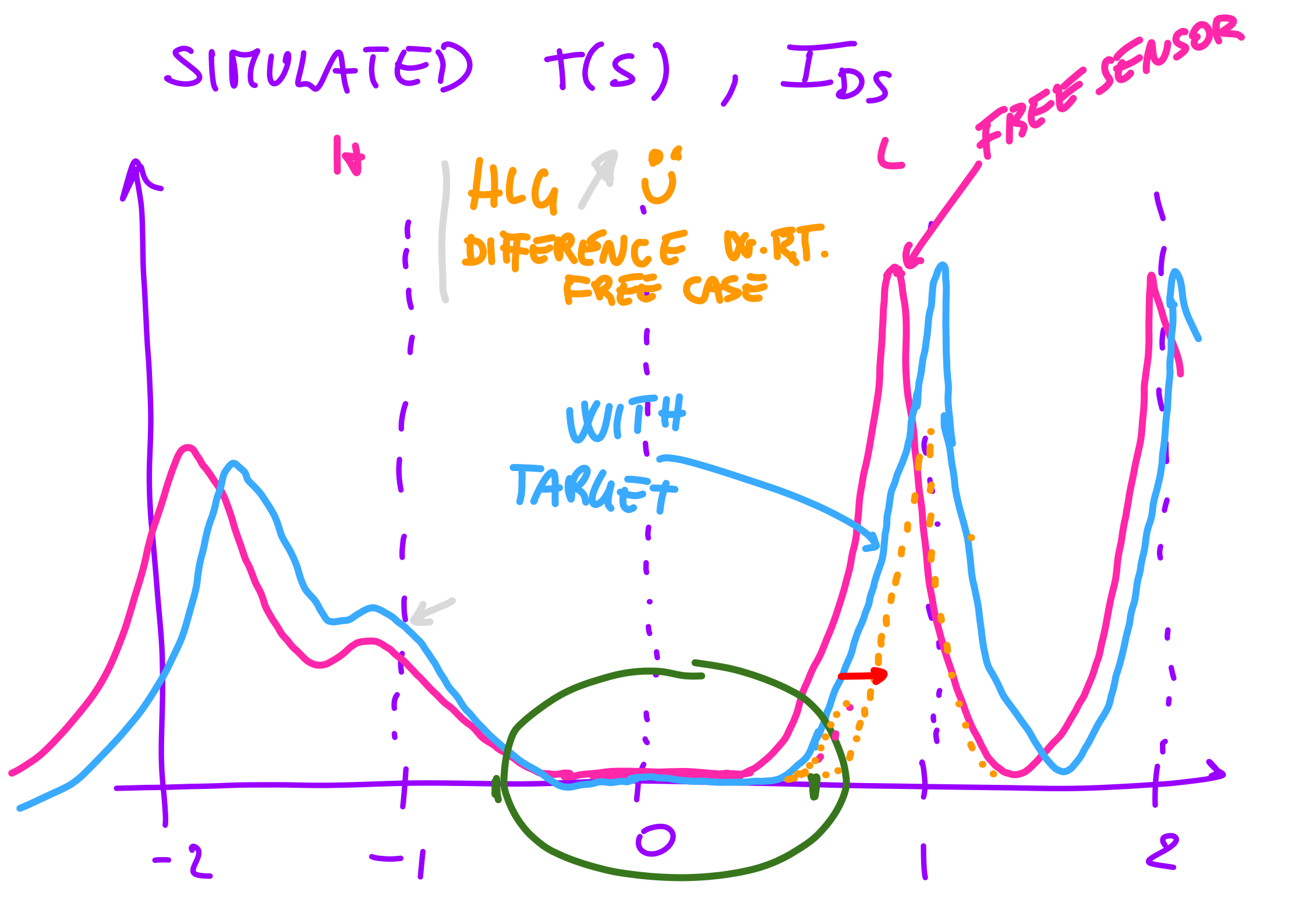
BASED PYRAMIDINE

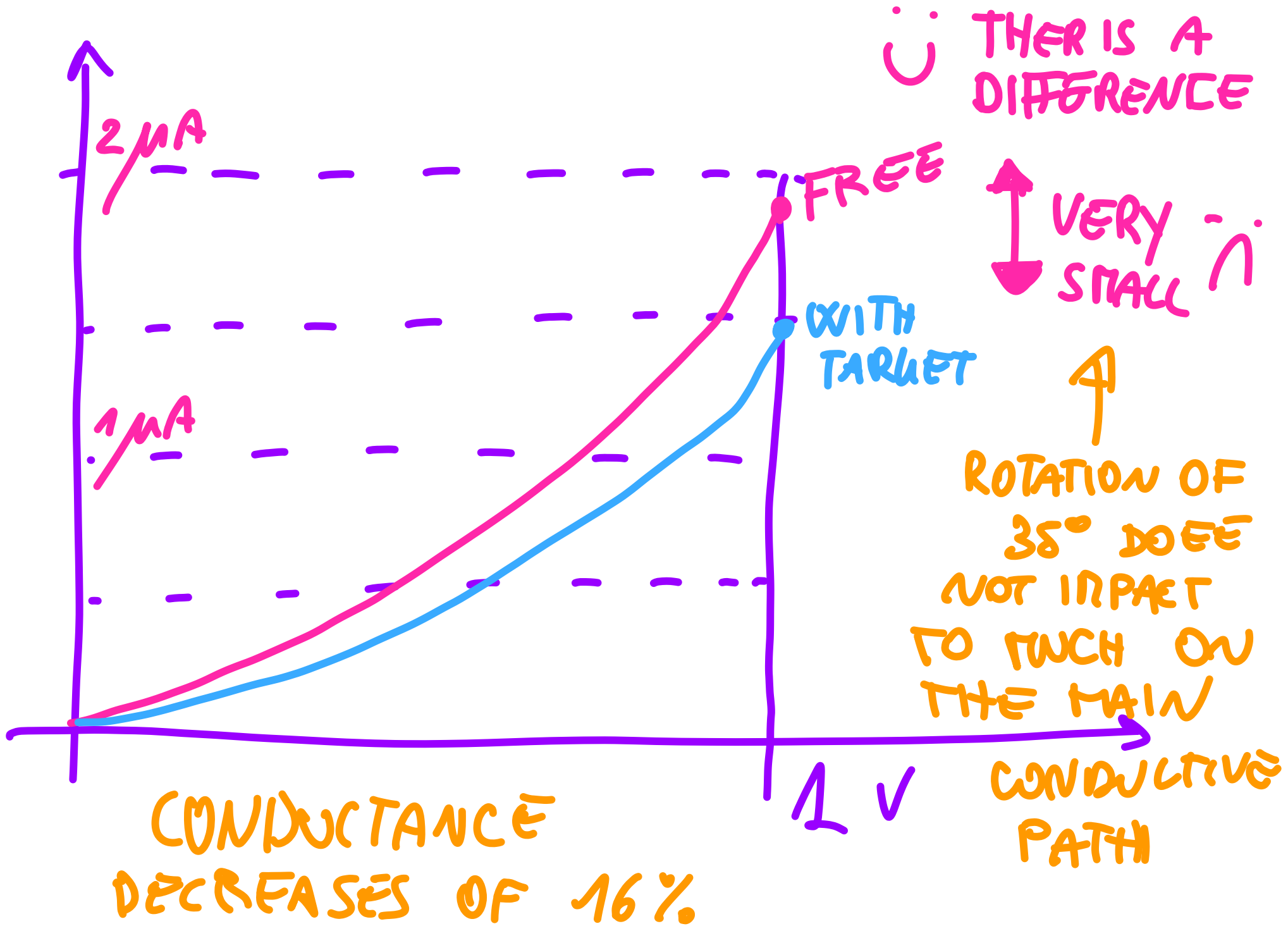




BOND TO DETECTION UNIT

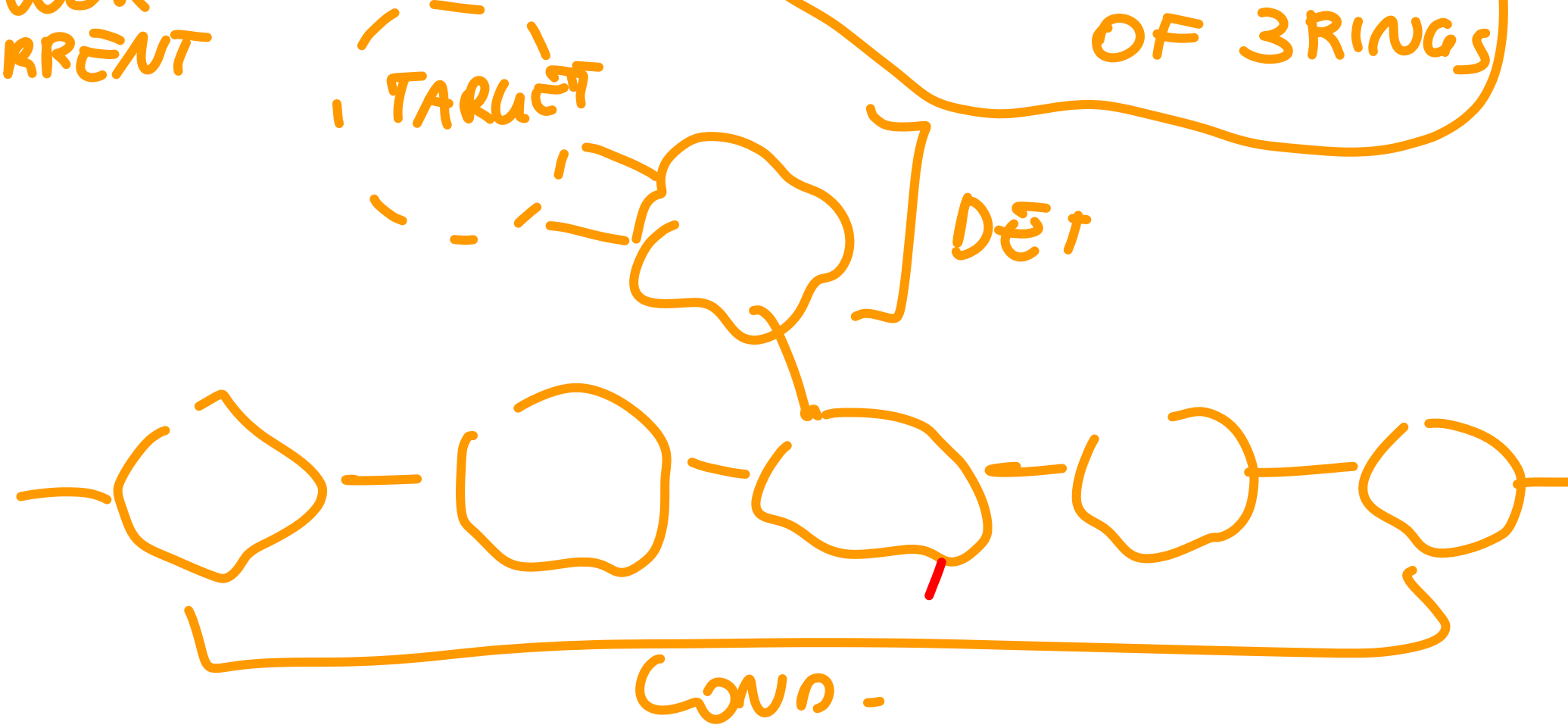

TOTAL COND + DET + TARGET
EXPECT REDUCTION CURRENT
CONJUGATED π BONDS LESS EFFECTIVE
DURING BONDING TO REACH MINIMUM ENERGY
TARGET + DET ROTATE 35° W.R.T. PLANE OF DET. UNIT
H BOND
H
O
N
C
N
C
C
H
H
C
H
H
O
H
N
H
H
C
N
H
N
C
D
S

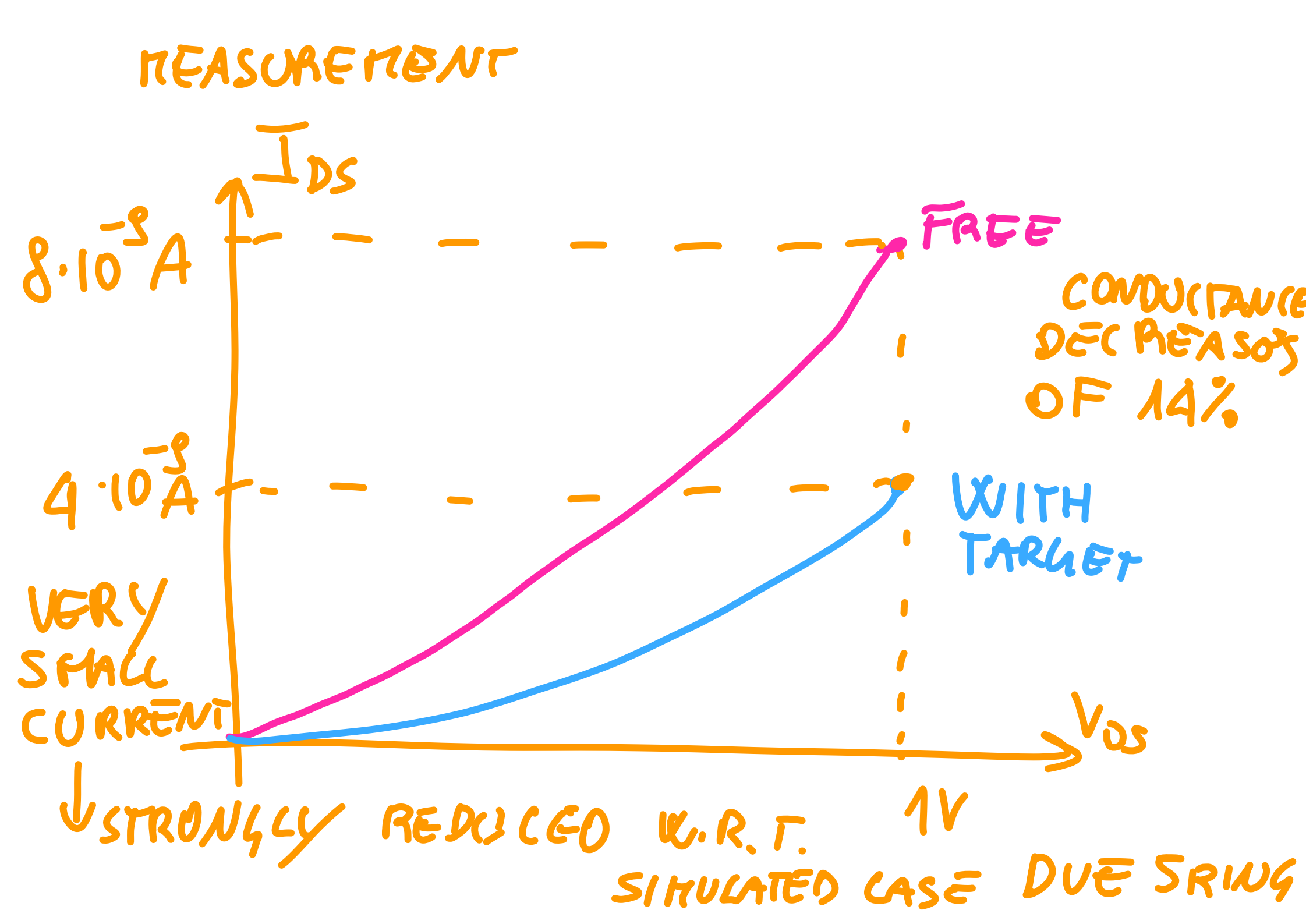

SIMULATED T(s), I_{DS}
H
L
HLG
DIFFERENCE W.RT. FREE CASE
FREE SENSOR
WITH TARGET
-2
-1
0
1
2


THERE IS A DIFFERENCE
2 μA
FREE
VERY SMALL
WITH TARGET
1 μA
ROTATION OF 35° DOES NOT IMPACT TO MUCH ON THE MAIN CONDUCTIVE PATH
1 V
CONDUCTANCE DECREASES OF 16%

EXPERIMENT → GAP NOT SO SMALL LENGHT OF ROPE HAD TO BE INCREASED 5 RINGS INSTEAD OF 3 RINGS

WE EXPECT LOWER CURRENT




MEASUREMENT
I_{DS}
$8 \cdot 10^{-9}$ A
$4 \cdot 10^{-9}$ A
FREE
CONDUCTANCE DECREASES OF 14%
WITH TARGET
VERY SMALL CURRENT
V_{DS}
1V
STRONGLY REDUCED W.R.T. SIMULATED CASE DUE SRING

OVERALL

→ VERY SMALL CURRENT (LENGTH) ☹

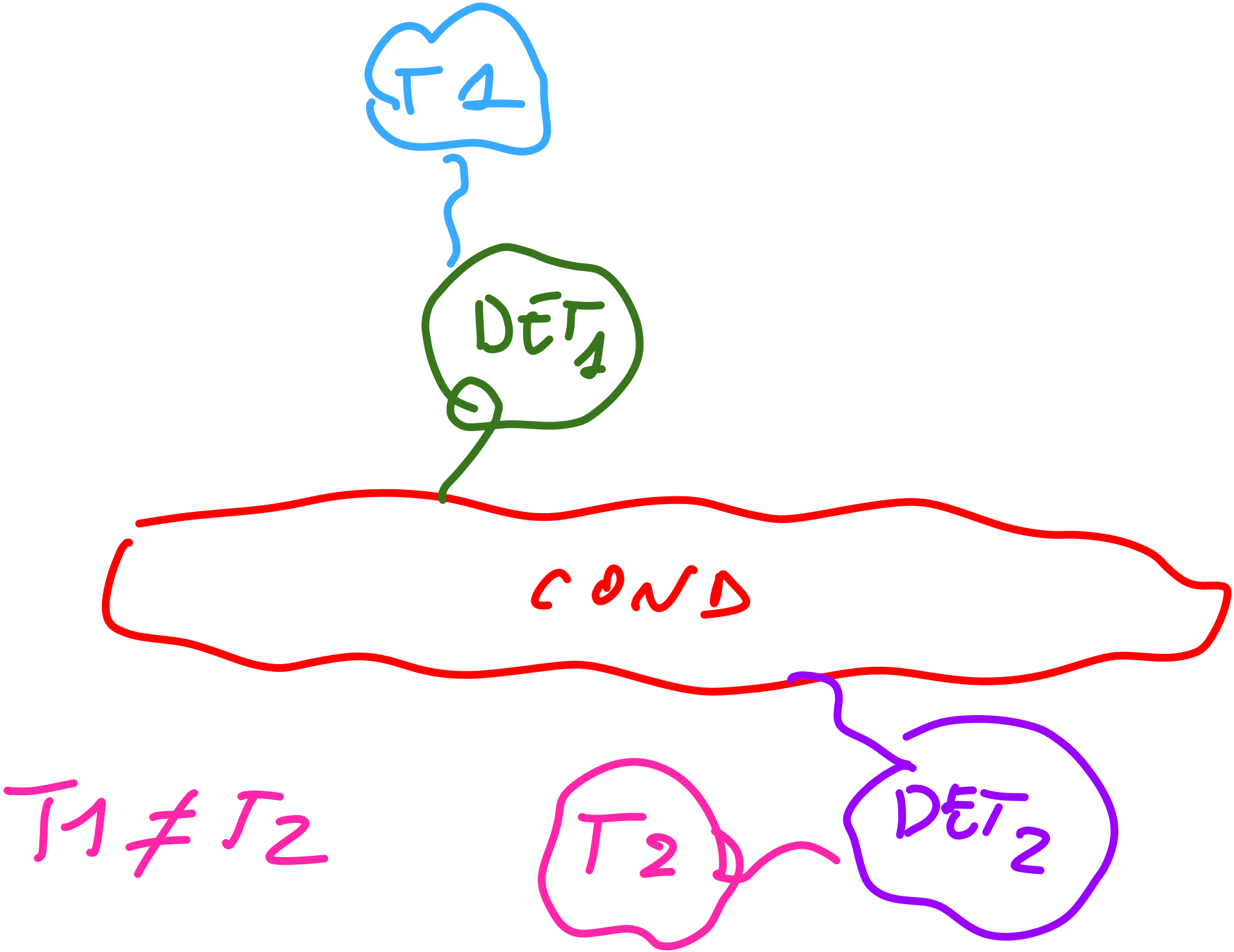
→ GAP HAS TO BE REDUCED

→ SMALL VARIATION FREE / WITH TARGET ☹

→ WE HAVE IT! ☺

- GAP REDUCED
- NO RINGS REDUCED
- H BONDS ? OTHER BONDS ?
  CHANGE DET. UNIT ?

INCREASE THE IMPACT ON THE MAIN PATH – CONDUCTION PATH


T1
DET1
COND
T1 ≠ T2
T2
DET2

CRISTALLIZATION

c) SME

d) SENSORS