M.T. BEHAVIOR & CHARACTERISTICS PART 2

M.T. BEHAVIOR

OBJECTIVES

a) PARAMETERS INVOLVED

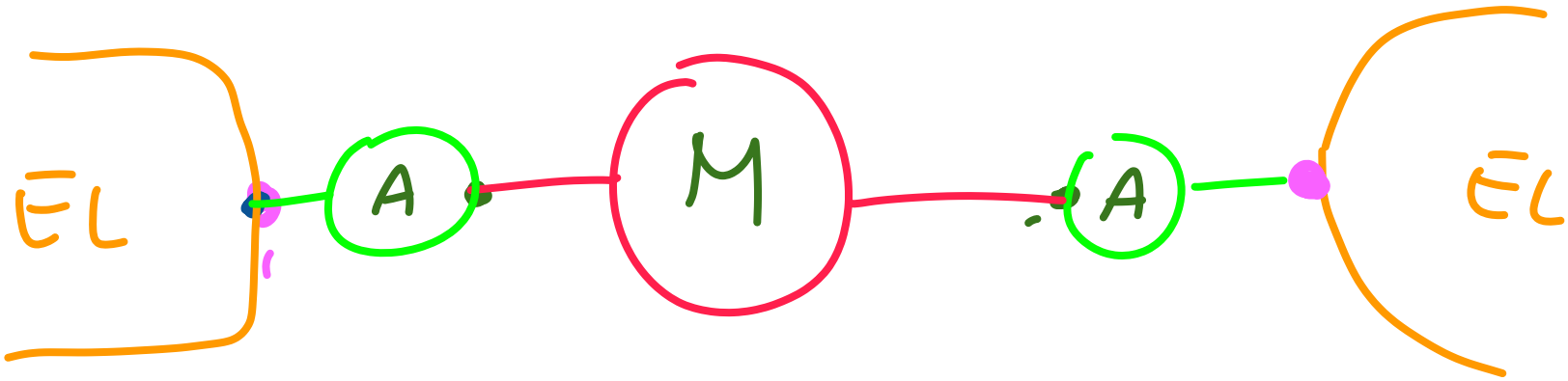
b) CHARGE SHARING, GATE

c) SCF LOOP

d) CIRCUITS

9) PARAMETERS INVOLVED

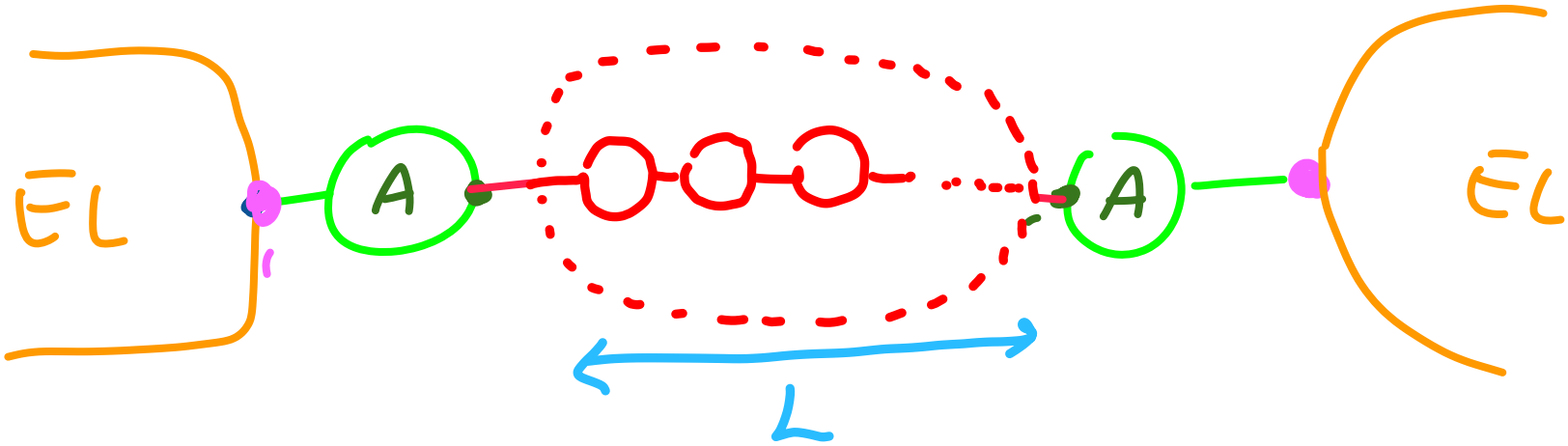
MOLECULAR TRANSISTOR



MAIN PARAMETERS

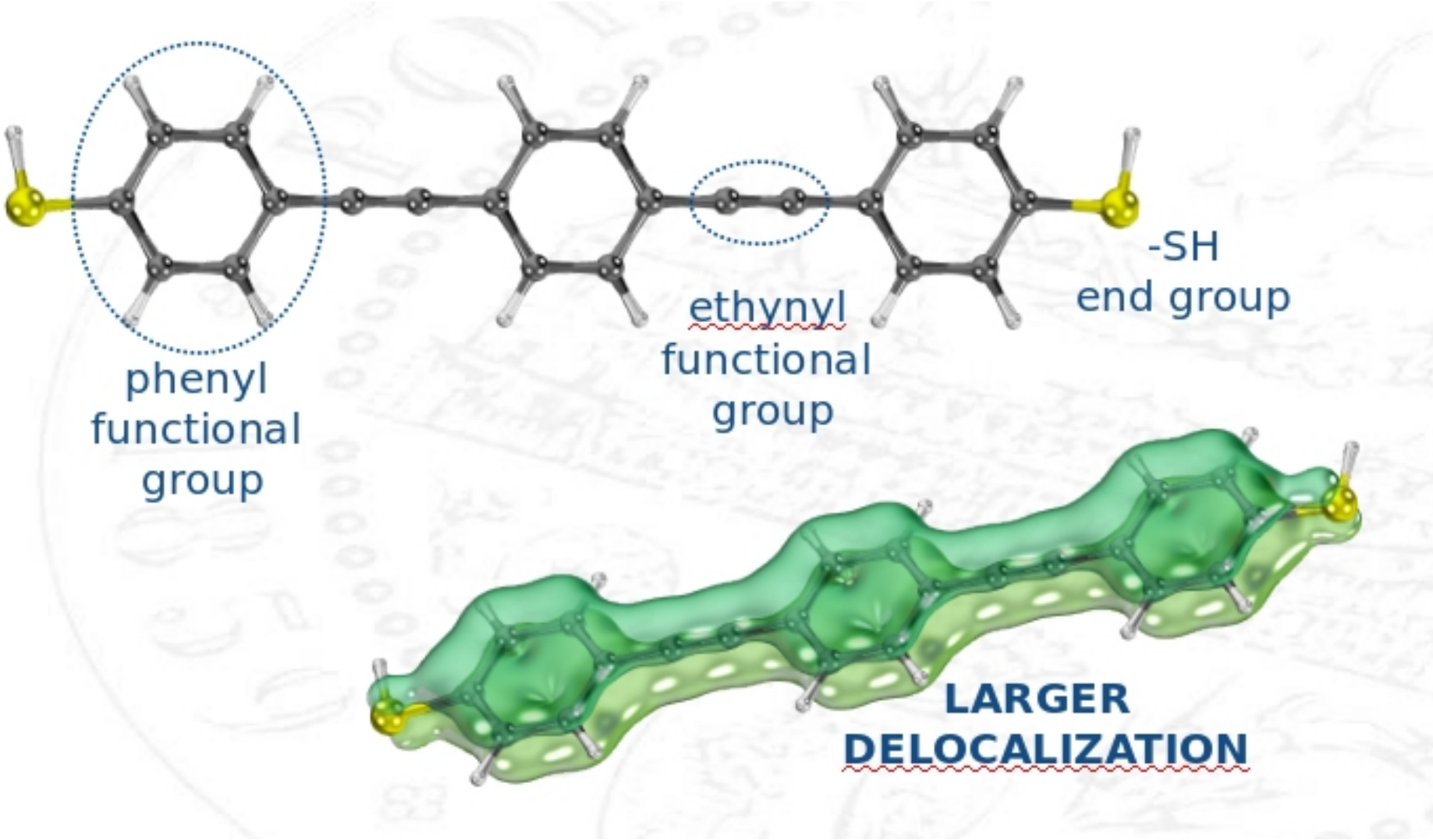
- MOLECULE LENGHT
- MOLECULE TORSION
- ANCHORING GROUP
- ELECTRODES

IMPACT OF LENGHT

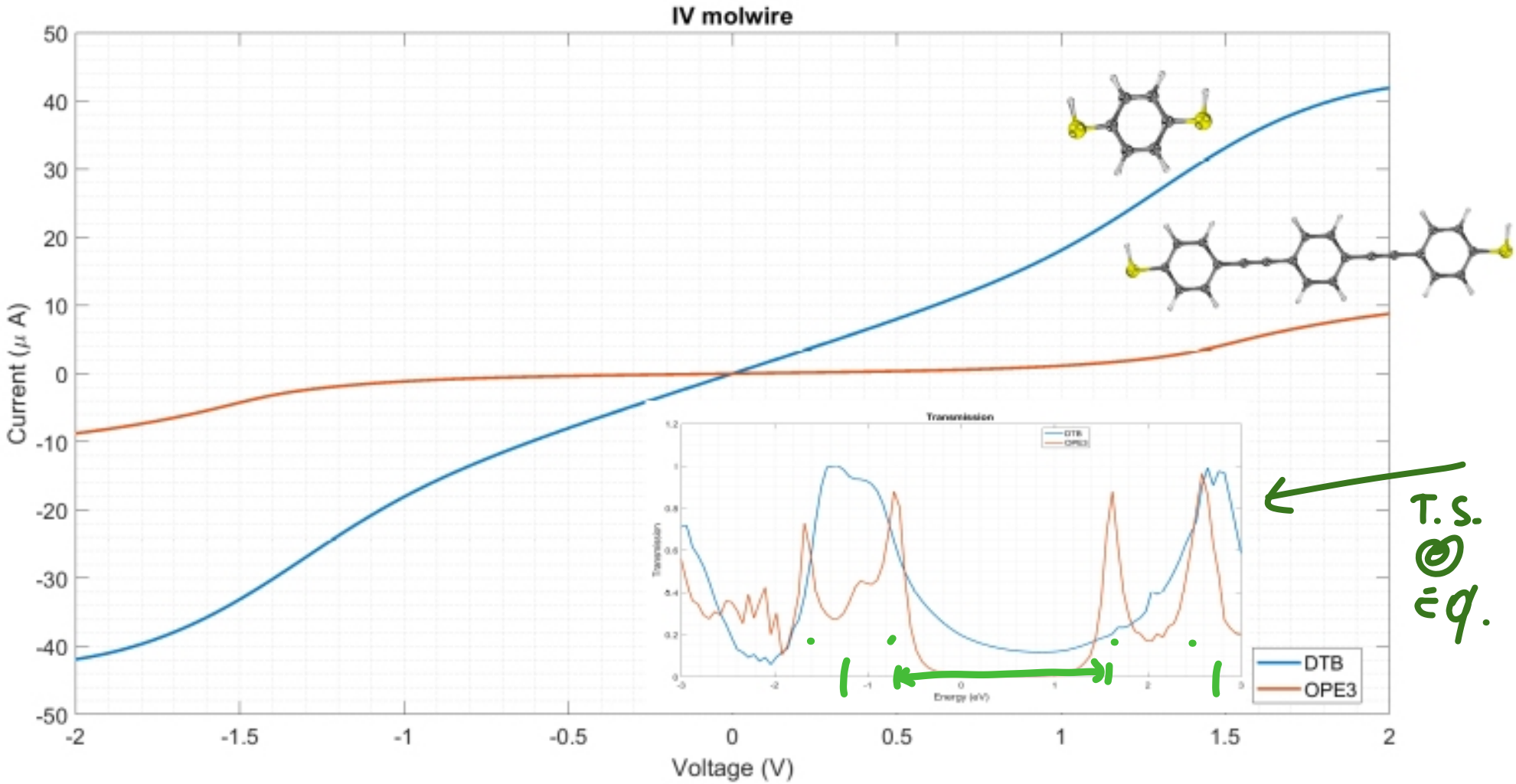


IN GENERAL IT MEANS A BIGGER NUMBER OF RINGS IN AROMATIC MOLECULES

LENGHT - EXAMPLE OPE3



TS AND I/V COMPARED : DTB vs OPE3



SIM. QUANTUM ATK

WHY?

WE EXPECT

MORE RINGS → MORE ATOMS → MORE ENERGY LEVELS

→ MORE CONDUCTIVITY → BIGGER CURRENT

BUT IF WE OBSERVE THE T(S)

MORE PEAKS AS EXPECTED, BUT NARROWER

→ LESS CHARGE → SMALLER CURRENT

NARROW PEAKS MEAN SMALLER BROADENING

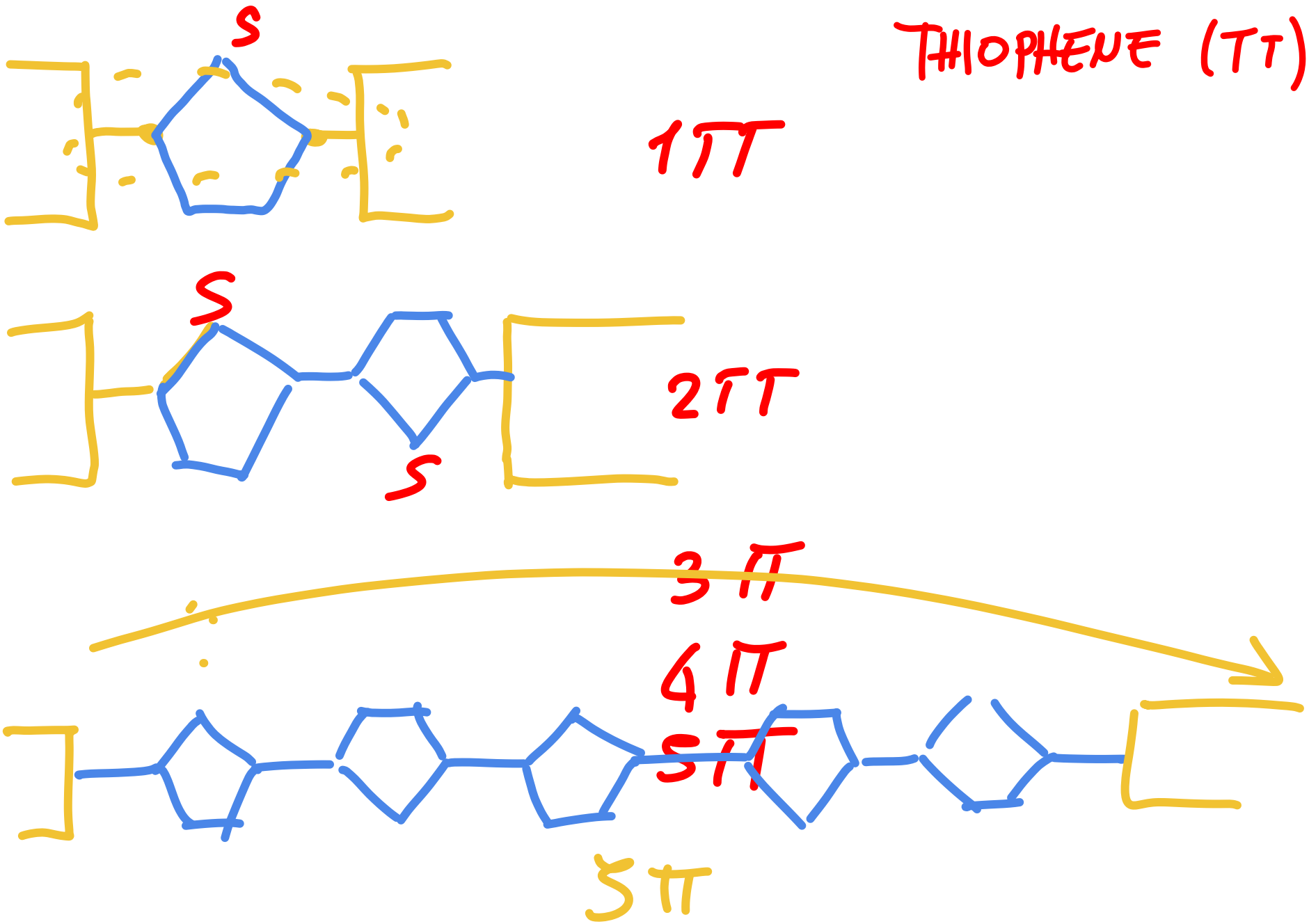
→ ↓ BW ELECTRODES AND MOLECULE IS REDUCED

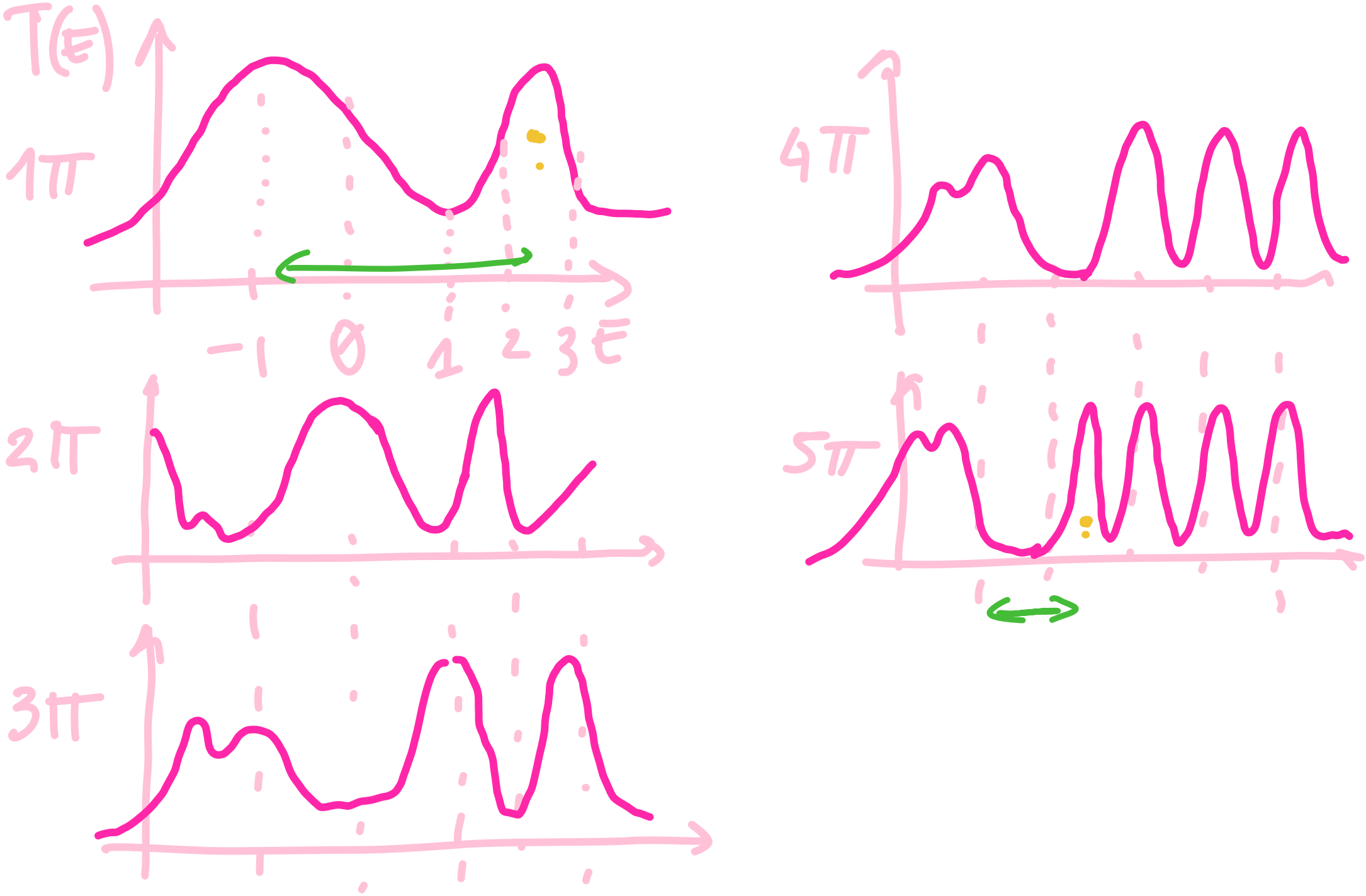
I.E. LARGER ELECTRODES SEPARATION → WEAK OVERLAP

BW. MOLECULE AND ELECTRODES STATES

DEPENDENCE ON LENGHT, ANOTHER EXAMPLE

THIOPHENE (Tt)




T(E)
1π
−1
0
1
2
3
E
2π
3π
4π
5π

WE OBSERVE

- **REDUCTION OF HLG** (2V for 1π, 1V for 5π)

  MORE RINGS → MORE STATES → HLG ↓ I ↗

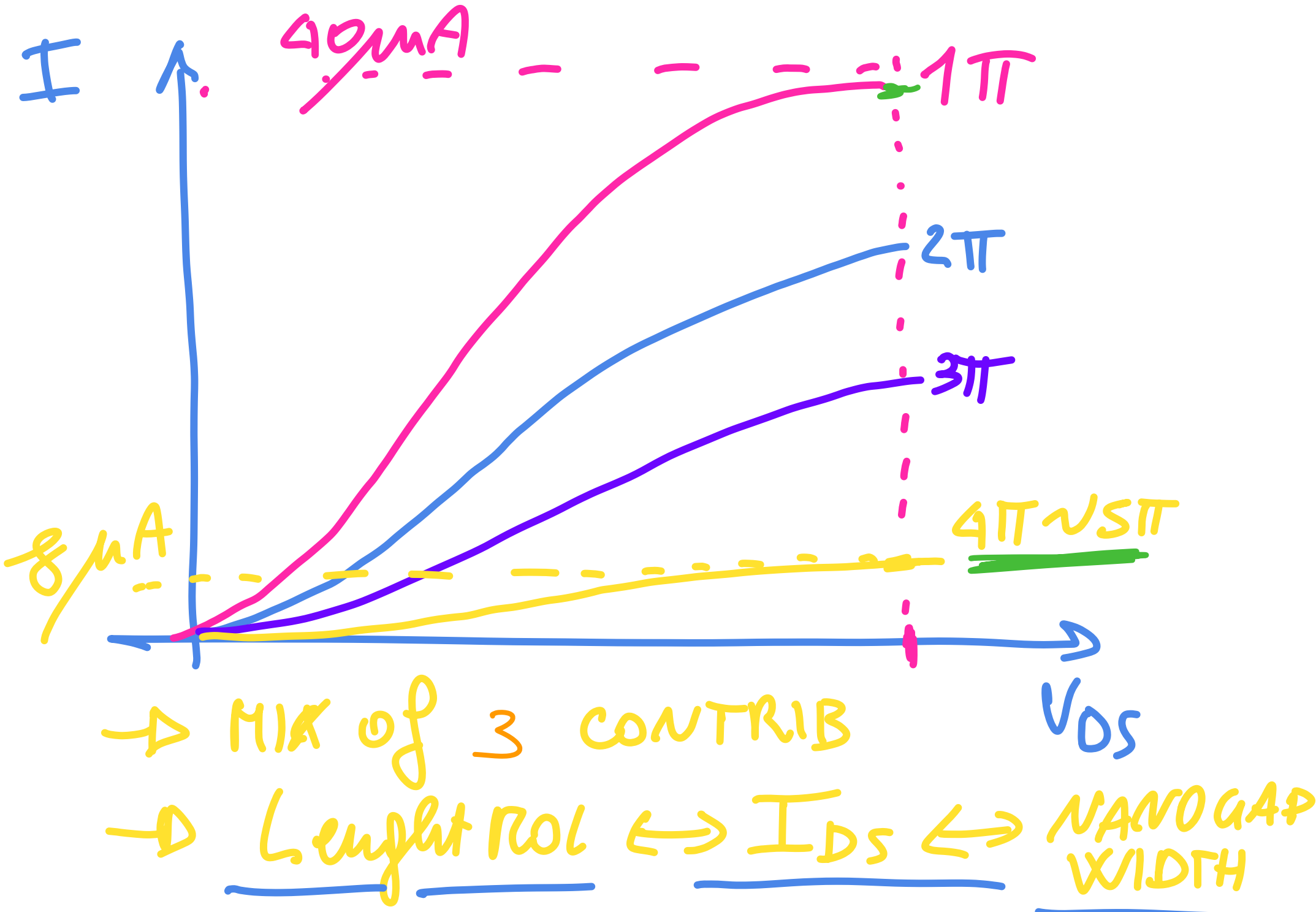
- **MORE PEAKS**

  LONGHER CHAIN → MORE ELECTRONS → MORE PEAKS

  I ↗

- **REDUCED BROADENING**

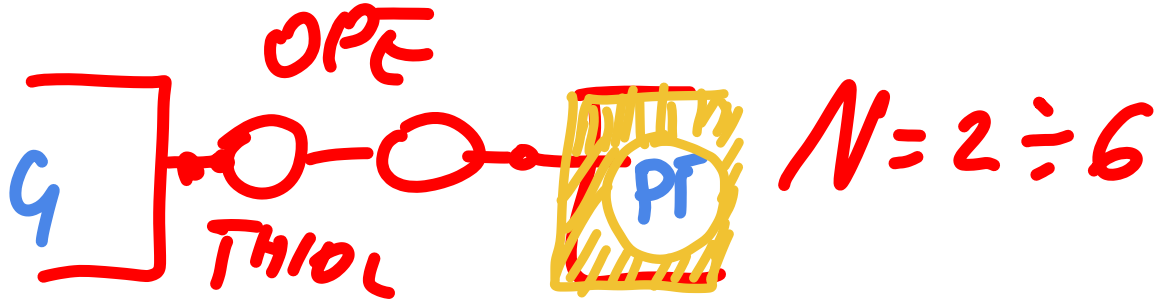
  MORE DISTANT ELECTRODES → WEAK OVERLAP BW MOL. & ELECTRODES → ∫ SMALLER → NARROWER PEAKS I ↘

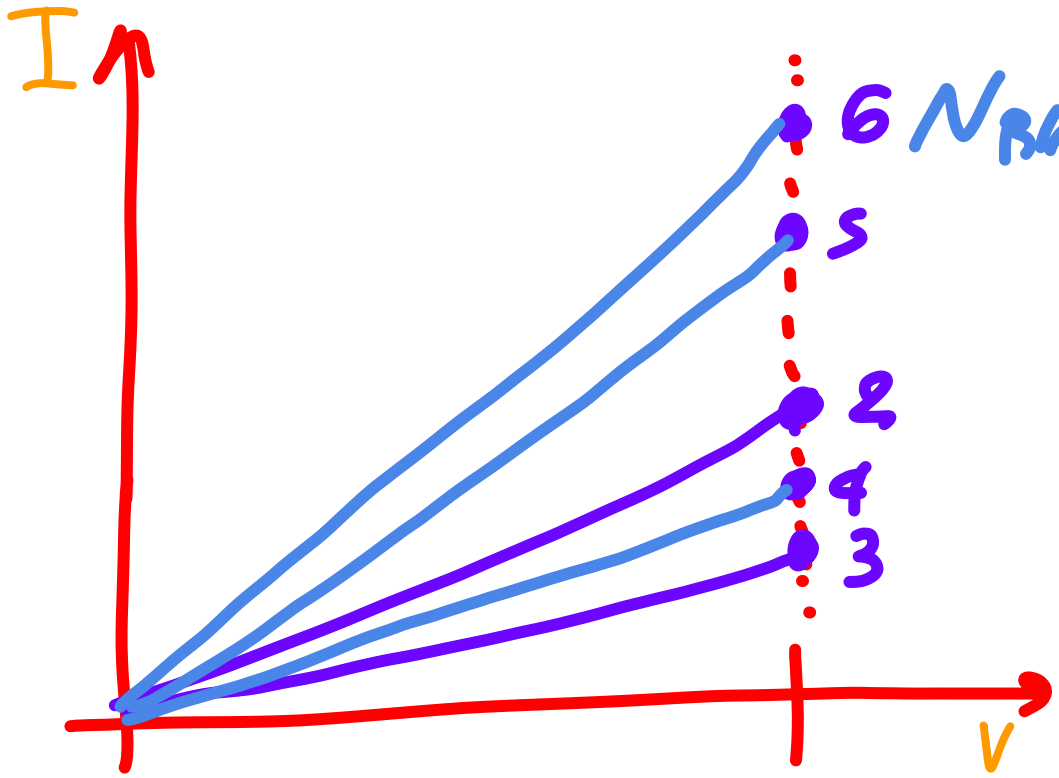


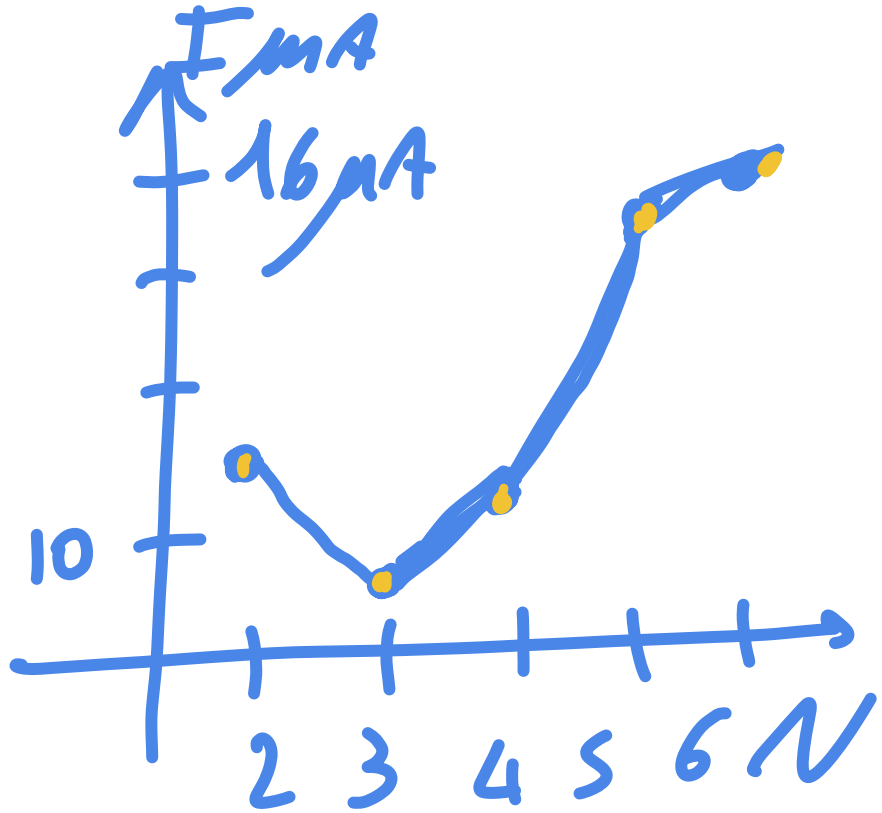
→ MIX of 3 CONTRIB

→ Lenght ROL ↔ I_{DS} ↔ NANOGAP WIDTH

ex OPE



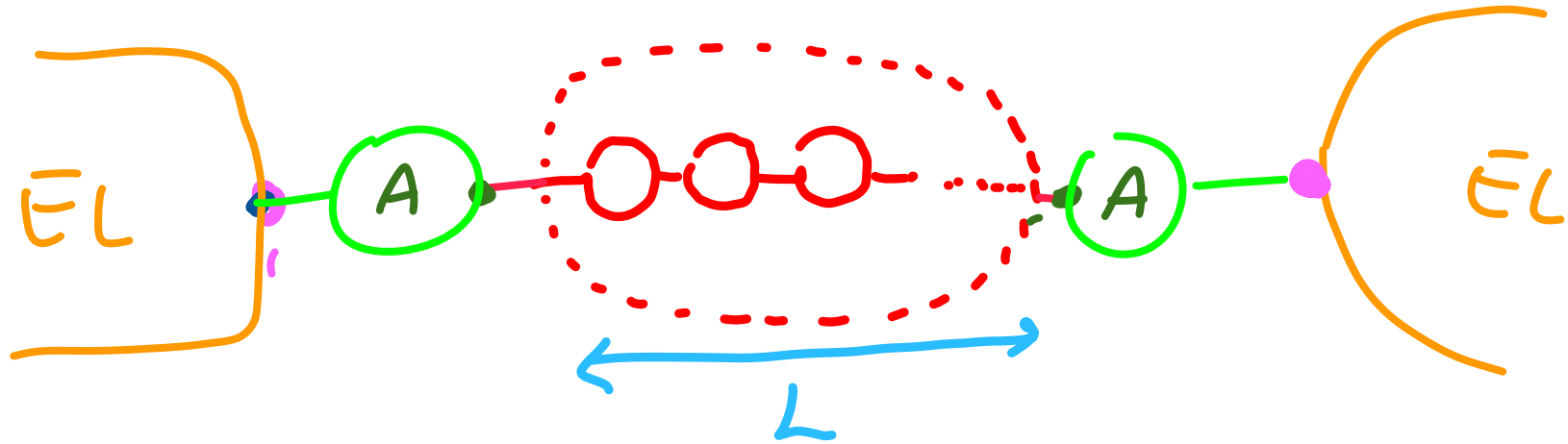




IN THIS CASE THE COMBINATION OF THE THREE CONTRIBUTIONS IS DIFFERENT DEPENDING ON THE N. OF RINGS

RECAP

MOLECULE LENGHT IMPACT ON CONDUCTION



1) REDUCED HLG 2) MORE PEAKS IN TS 3) REDUCED BROADENING

I_{DS} DEPENDS ON HOW 1,2,3 COMBINE

WHAT WE LEARN:

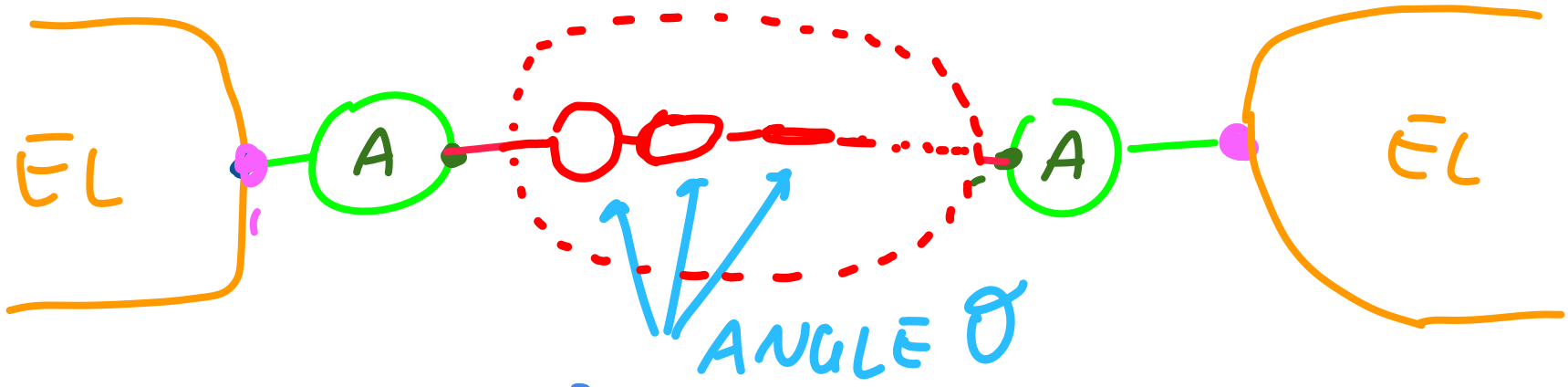
① IN CASE OF A TECH WHERE THE NGAP WIDTH IS FIXED THE LENGHT OF THE MOL. MUST BE CHOSEN ACCORDINGLY AND THE CONSEQUENCES IN TERMS OF CURRENT HAVE TO BE CONSIDERED → AN OPTIMAL MOL. SHOULD BE SELECTED

(2) IN CASE THE GAP WIDTH CAN BE CONTROLLED THEN THE RELATION WILL BE

→ DECIDE THE TOL & TOL. LENGHT

→ TRIM THE GAP AS A CONSEQUENCE

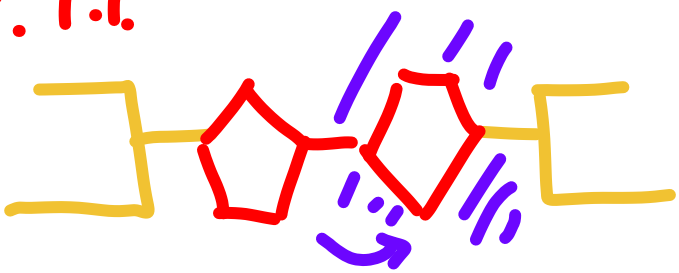
EFFECT OF TORSION



- DUE TO FREEDOM IN RINGS CONNECTION POINTS IN SOME MOLECULES

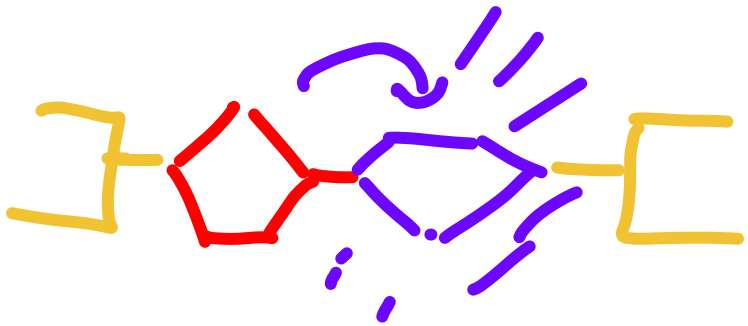
- INFLUENCED BY THE PROCESS OF ATTACHMENT AND BONDING TO ANCHORING AND GATES

ex. T.T.

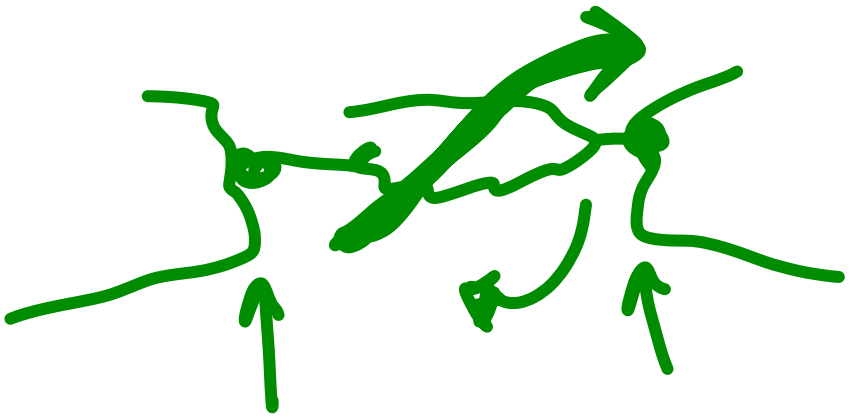


2 RINGS IN SAME PLANE

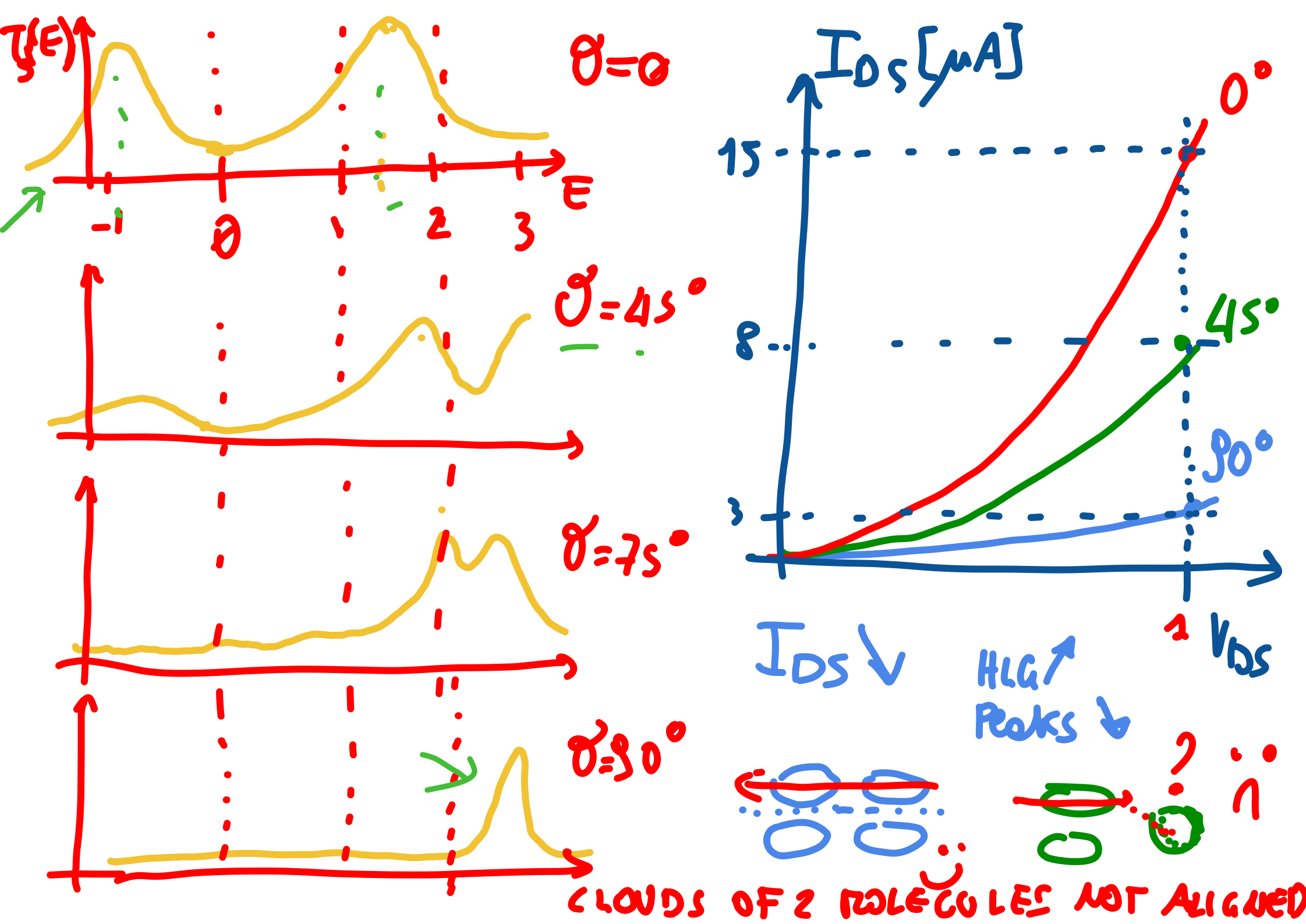
$\theta = 0°$



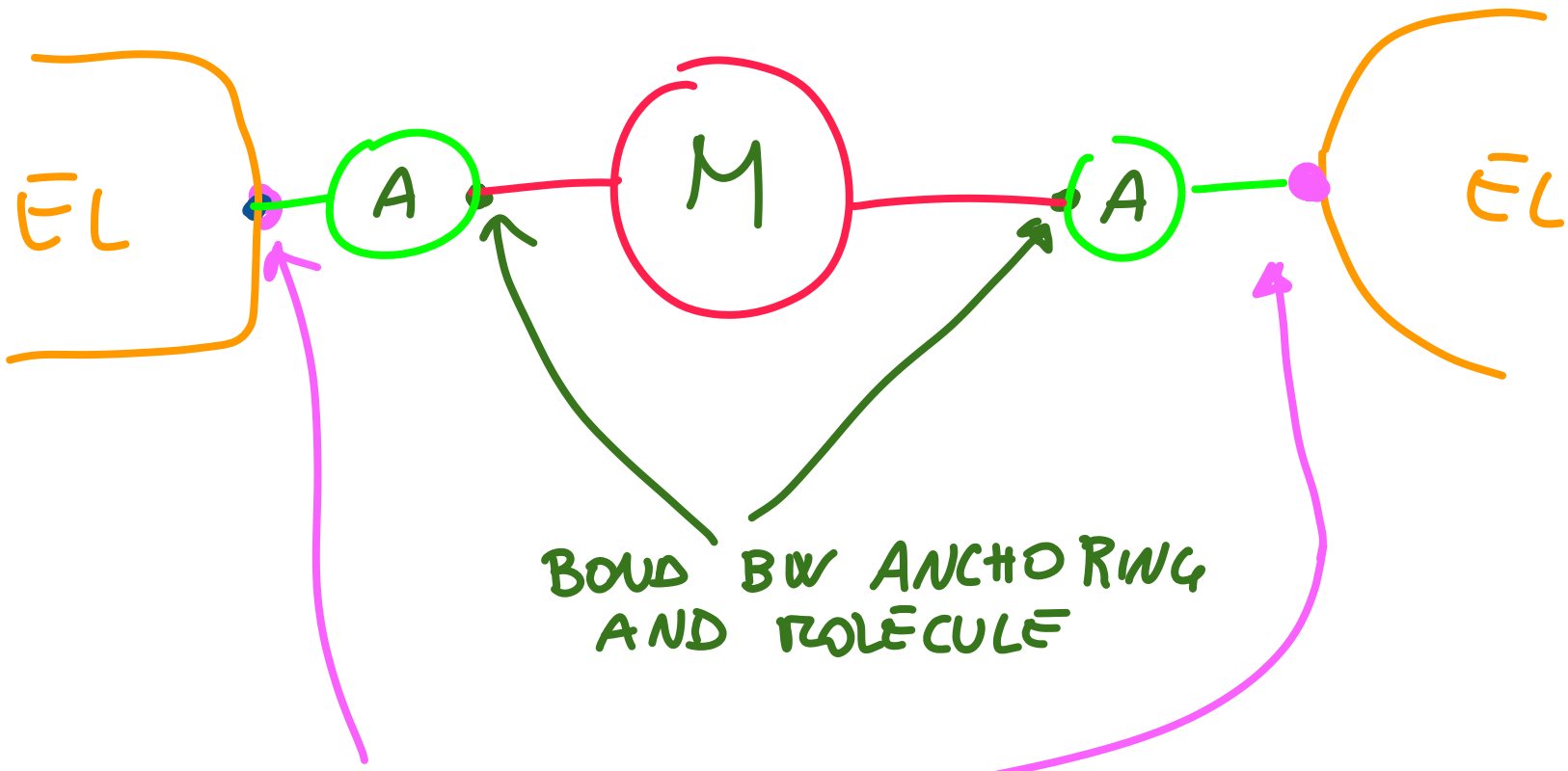
θ ROTATED 45°, 75°, 90°



TORSION MIGHT HELP BONDS CREATION

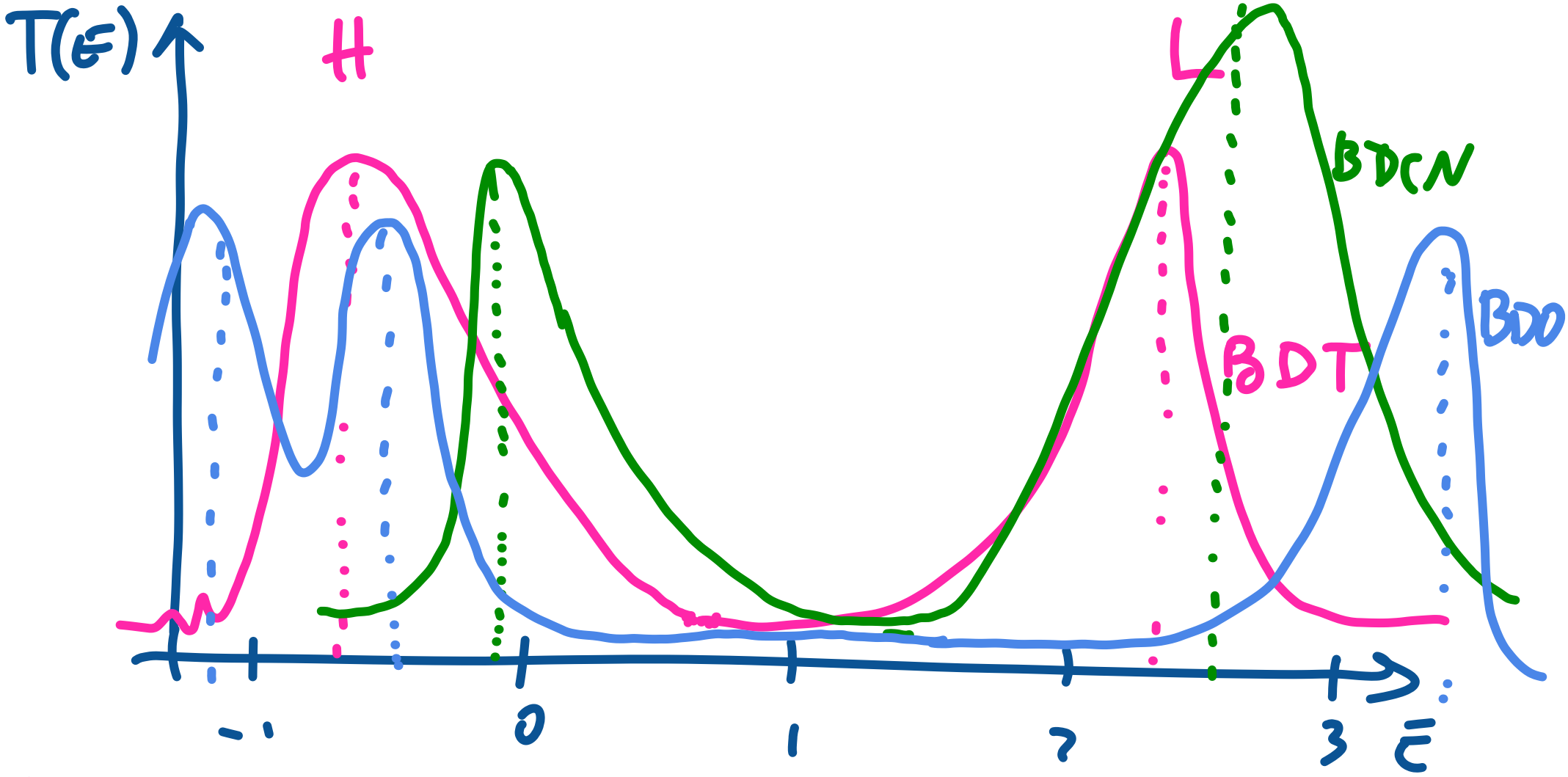

T(E)
E
-1
0
2
3
θ=0
θ=45°
θ=75°
θ=90°
I_DS [μA]
15
8
3
0°
45°
90°
1
V_DS
I_DS ↘
HLG ↗
Peaks ↘
CLOUDS OF 2 MOLECULES NOT ALIGNED

DEPENDENCE ON TYPE OF ANCHORING GROUP (LINKER)

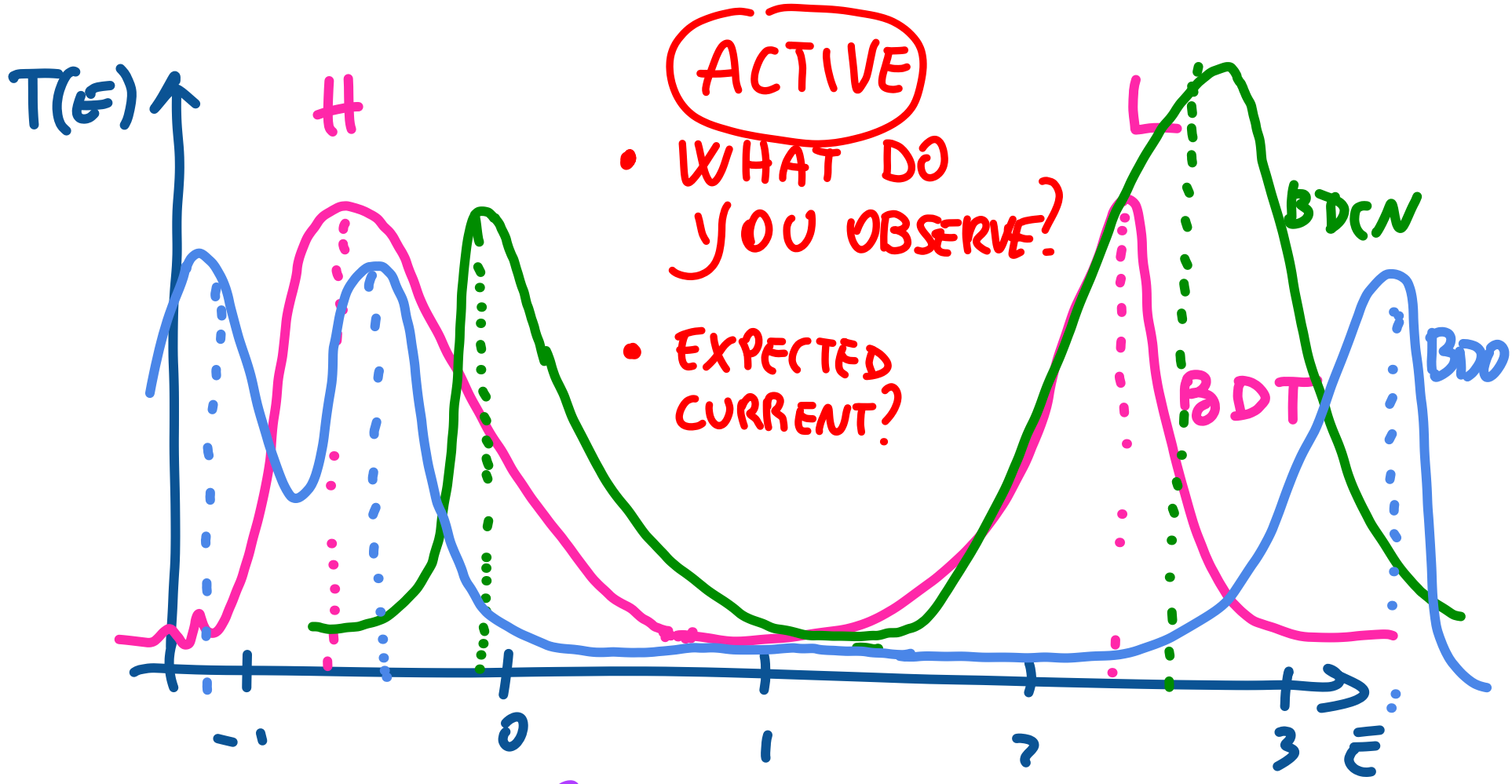


3 CASES: THIOL (-SH), CYANIDE (-CN), OXIGEN (-O)

DEPENDENCY ON ANCHORING GROUPS



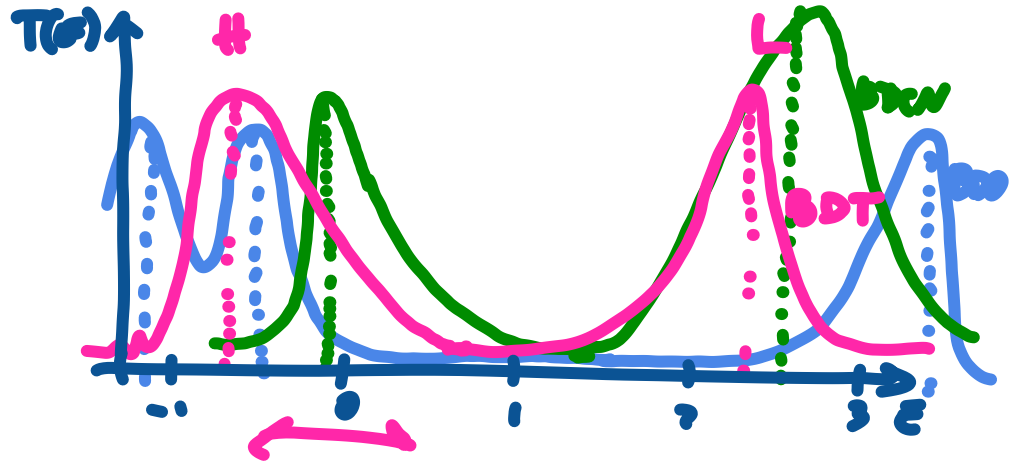
BDT - BENZENE DI THIOL
BDCN - BENZENE DI CYANIDE $C \equiv N$
BDO - BENZENE DI OXYGEN



BDCN vs BDT ?

BDO Vs BDT ?

BDO vs BDCN ?



VERY HIGH DIFFERENCE!

WHY?

[μA]

I_{DS}

4.5

2.5

2

BDCN

BDT

BDO

SMALLER

WHY?

0.5

1

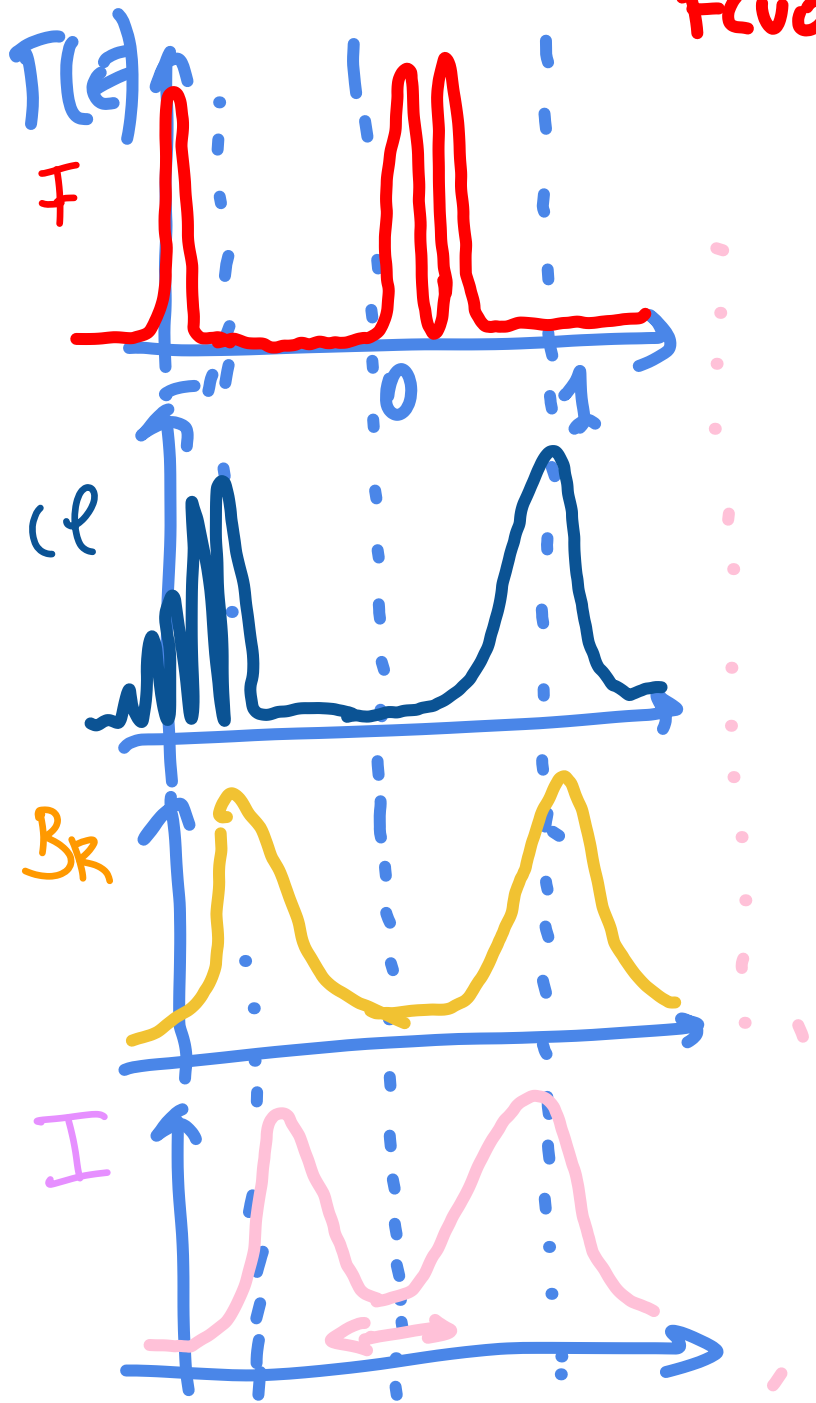
1.5

[V]

V_{DS}

BENZENE + F FLUORINE, Cl CHLORINE, Br, I

4 3 2.8 2.5 E_N



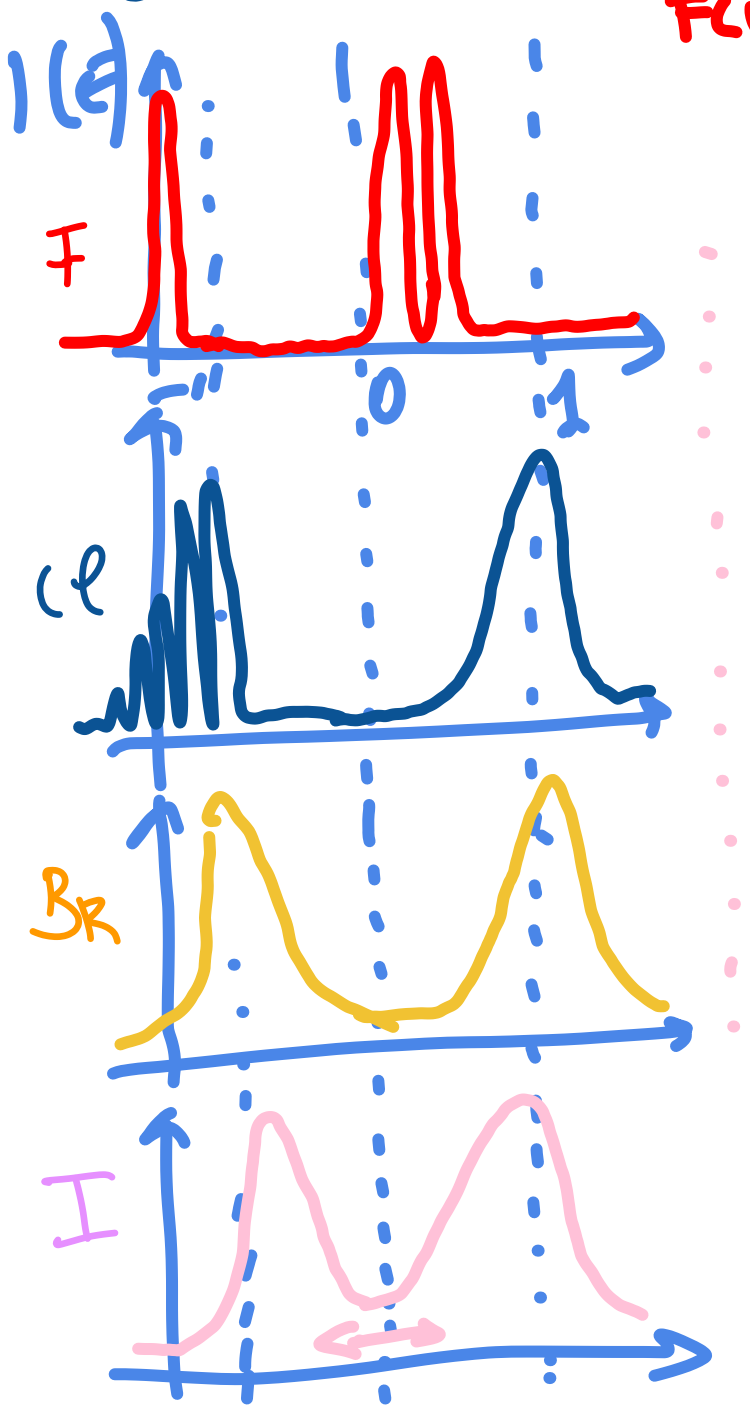
E_N = ELECTRONEGATIVITY, i.e. HOW MUCH ELECTRONS ARE ATTRACTED

E_N ↗ HIGH ATTRACTION

← if E_N ↗

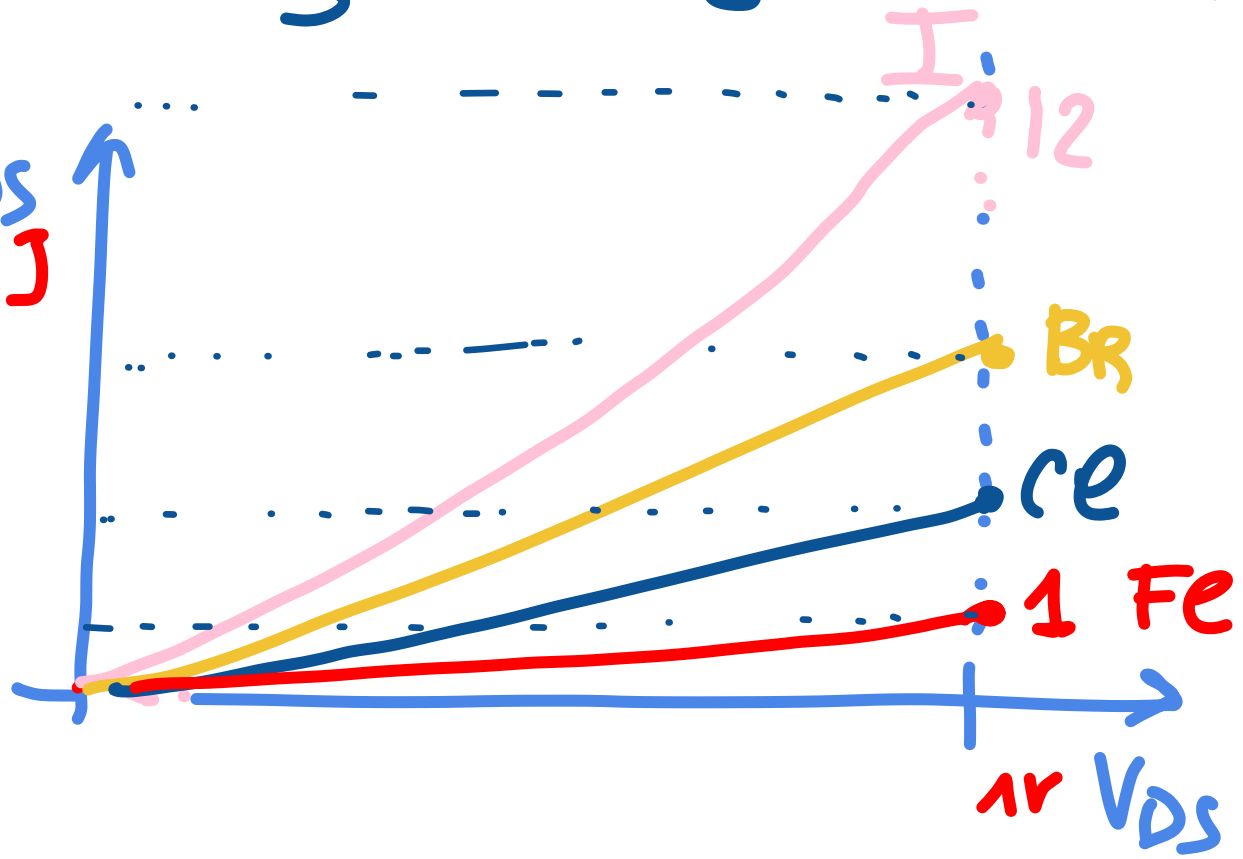
- HLG DECCREASES
- BROADENING DECREASES
- N. OF PEAKS INCREASES

BENZENE + F FLUORINE, Cl CHLORINE, Br, I



F	Cl	Br	I
4	3	2.8	2.5

E_M

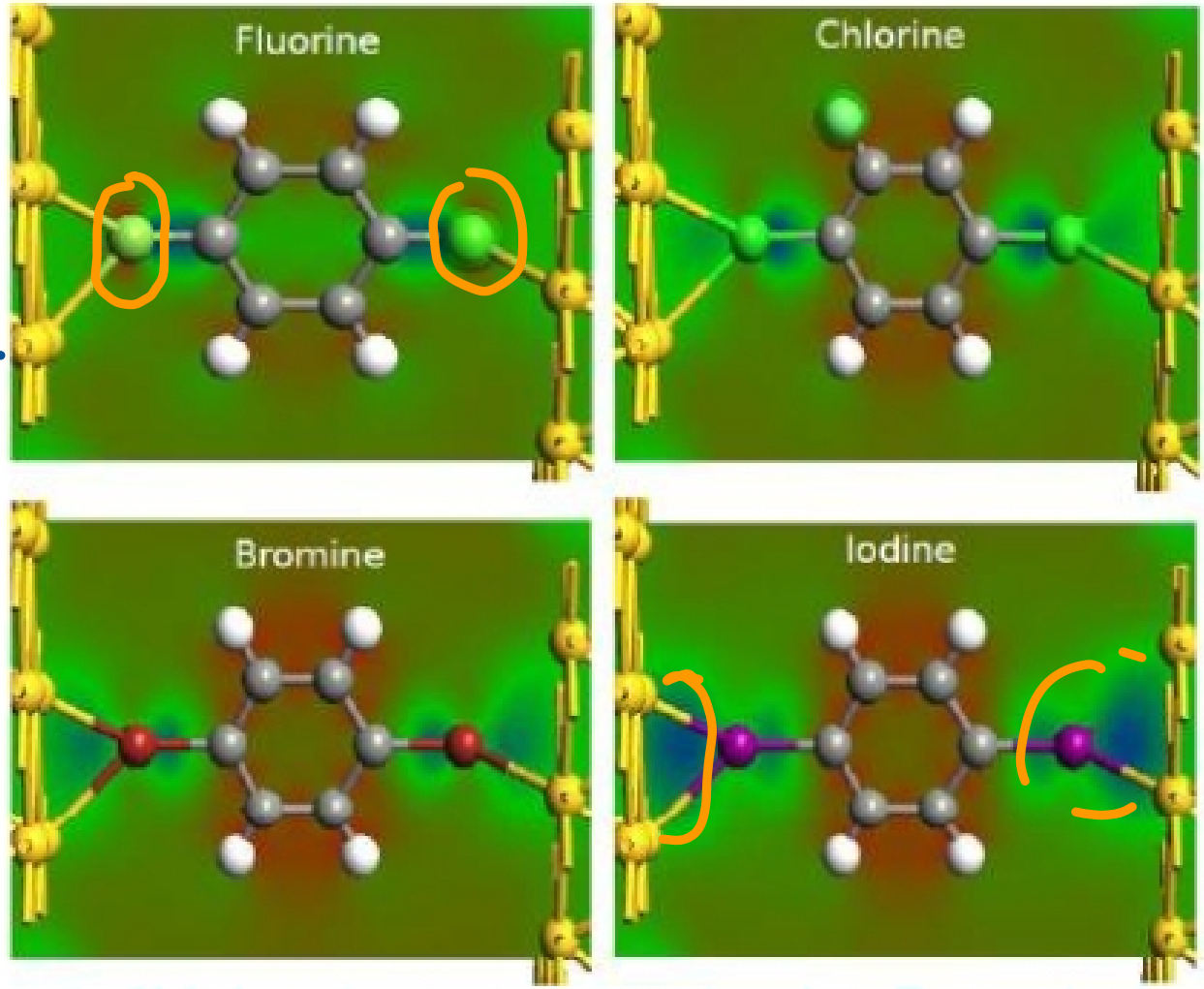


E_N = ELECTRONEGATIVITY, i.e. HOW HUCH ELECTRONS ARE ATTRACTED

E_N ↗ HIGH ATTRACTION

POTENTIAL ENERGY DISTRIBUTION IN SPACE 3D

HIGH E_N
MORE NEGATIVE CHARGE NEAR ELECTR.
↓
HIGH BARRIER
↓
LOW BROADENING



HIGH POT. ENERGY → RED

LOW POT. ENERGY → BLU

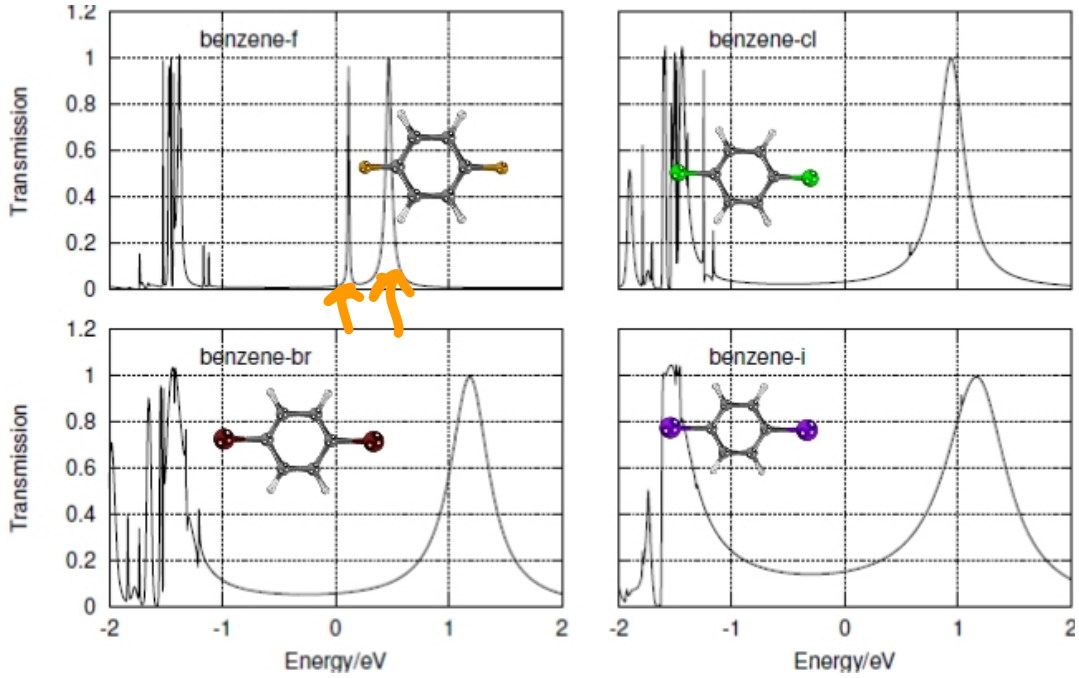
← POTENTIAL LESS AROUND LINKERS
· BETTER COUPLING
MORE BROADENING

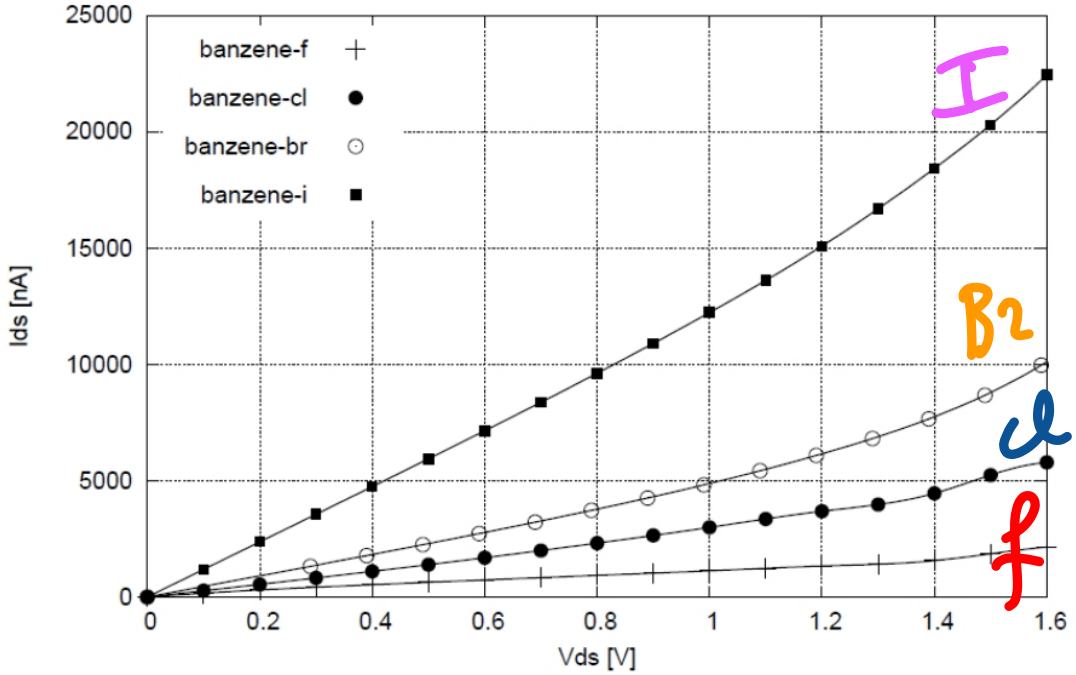
Zahir *et al.*, "Molecular transistor circuits: From device model to circuit simulation," *2014* 10.1109/NANOARCH.2014.6880492.

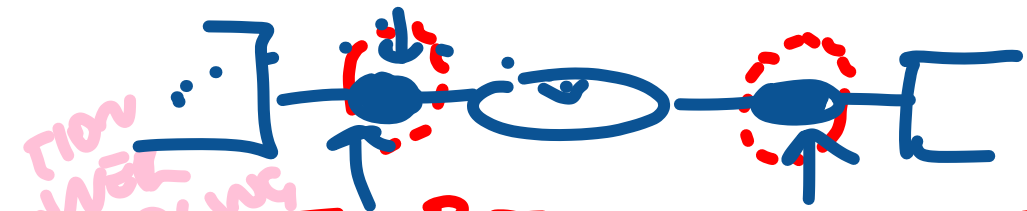
MORE ELECTRONEGATIVE LINKERS ATTRACT MORE THE ELECTRONS THAT "STAY" THERE → REPULSIVE FOR NEW EL.!

BENZENE + F FLUORINE, Cl CHLORINE, Br, I

9 3 2.8 2.5 EN







1V DS

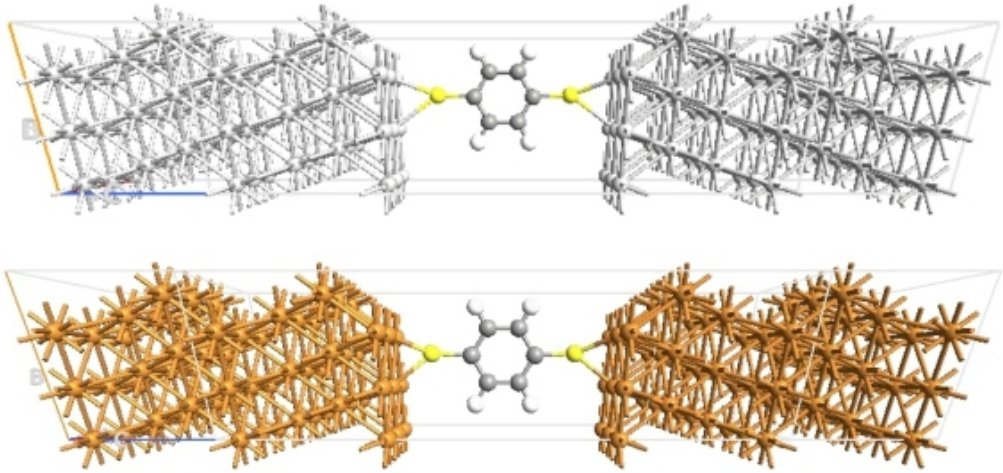
ION WIRE COUPLING

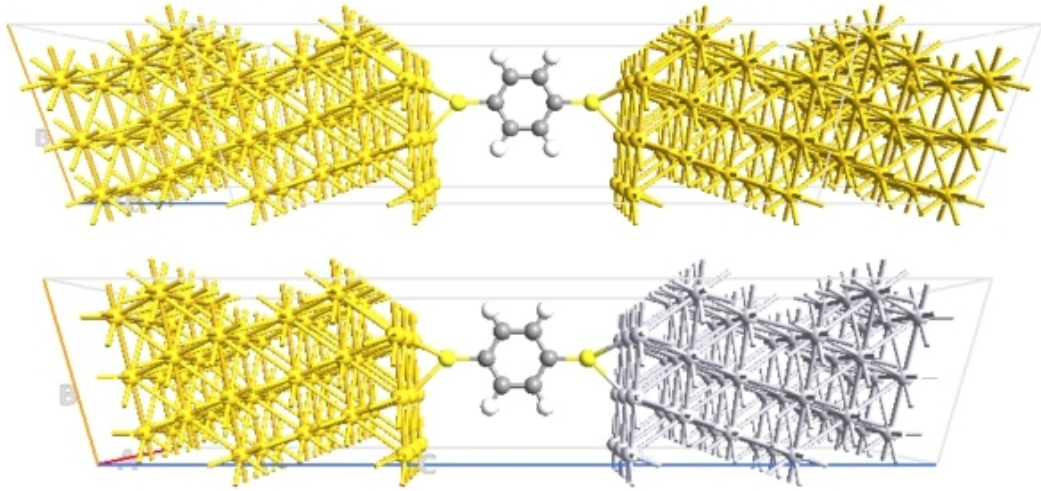
Es POTENTIAL CONCENTRATED AROUND ANC. GROUPS

→ ELECTR. TRAPPED CREATE BARRIERS

IMPACT OF ELECTRODES

ACT AS CHARGE RESERVOIR

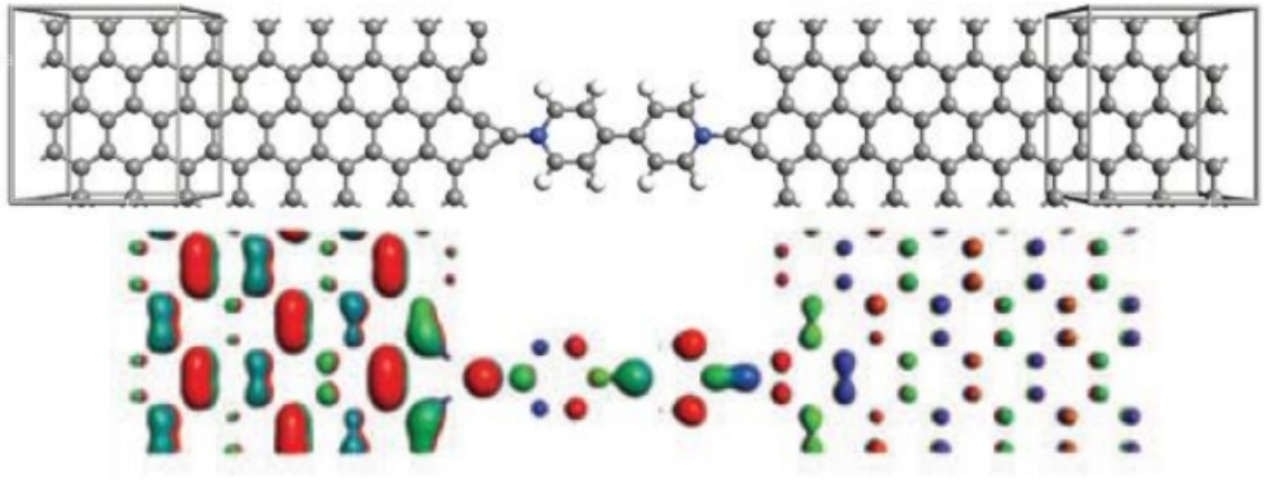




- NORMALLY NOBLE METALS ARE USED
- INFLUENCE THE ANCHORING
- IMPACT ON BROADENING
- DIFFERENT METALS FOR D & S → FAVOUR RECTIFICATION (DIODE)

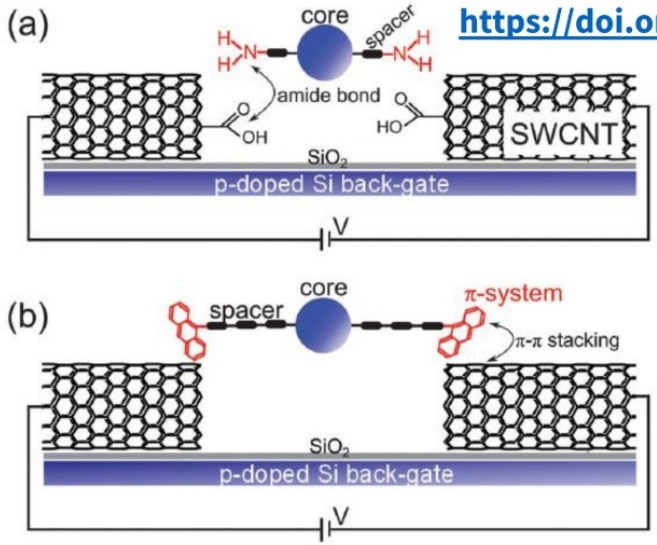
RECENTLY CARBON BASED ELECTRODES ARE INVESTIGATED

GRAPHENE



Li et al (2016). Distinctive Electron Transport on Pyridine-Linked Molecular Junction with Narrow Monolayer Graphene Nanoribbons 18. 10.1039/C6CP05007G.

CARBON NANOTUBES



https://doi.org/10.1039/C4CS00231H

CRISTALLIZATION

→ IDS FOR MOL. WIRE FROM TS TO IV

→ DEPENDENCY ON PARAMETERS

- LENGHT
- TORSION
- ANCHORING GROUP
- ELECTRODES