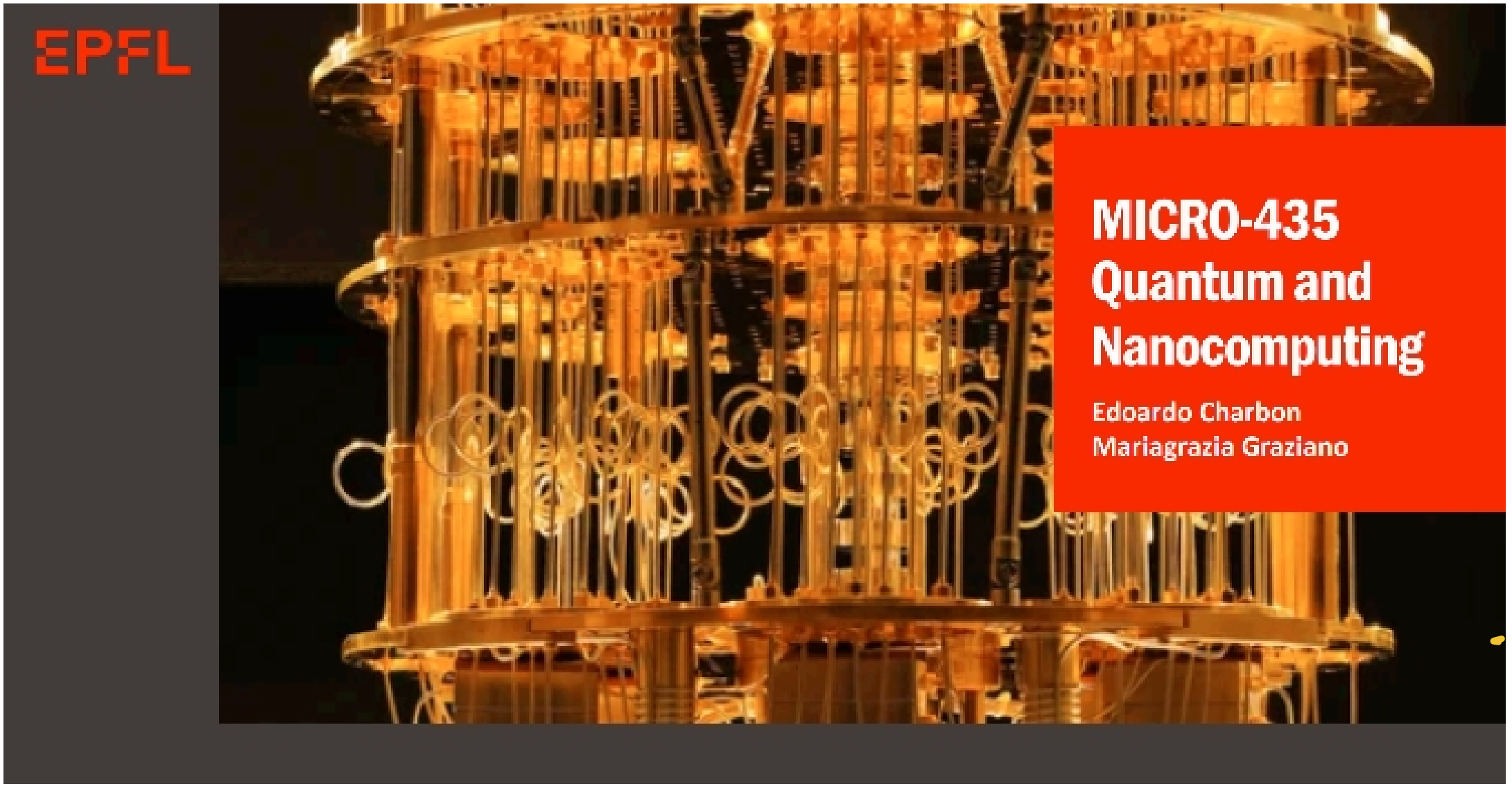


MOLECULES: AN OVERVIEW

11-12/11/25

REVIEW OF HYDROCARBONS

AND A VIEW ON THE MAIN MOLECULES USED IN THIS COURSE

CARBON

ELECTRONS DISTRIBUTION

$Z = 6$

ATOMIC NUMBER

2 EL. ON ORBITAL

$1s^2$

2 EL ON ORBITAL

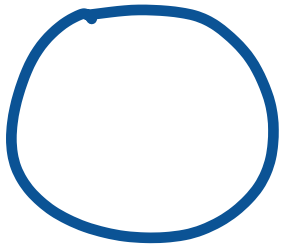
$2s^2$

2 EL ON

p_x p_y

$2p^2$

OPPOSITE SPIN



S TYPE

p TYPE

HYDROCARBONS

H + C

FORM EASILY STABLE CHAINS

WITH SINGLE / DOUBLE / TRIPLE BONDS

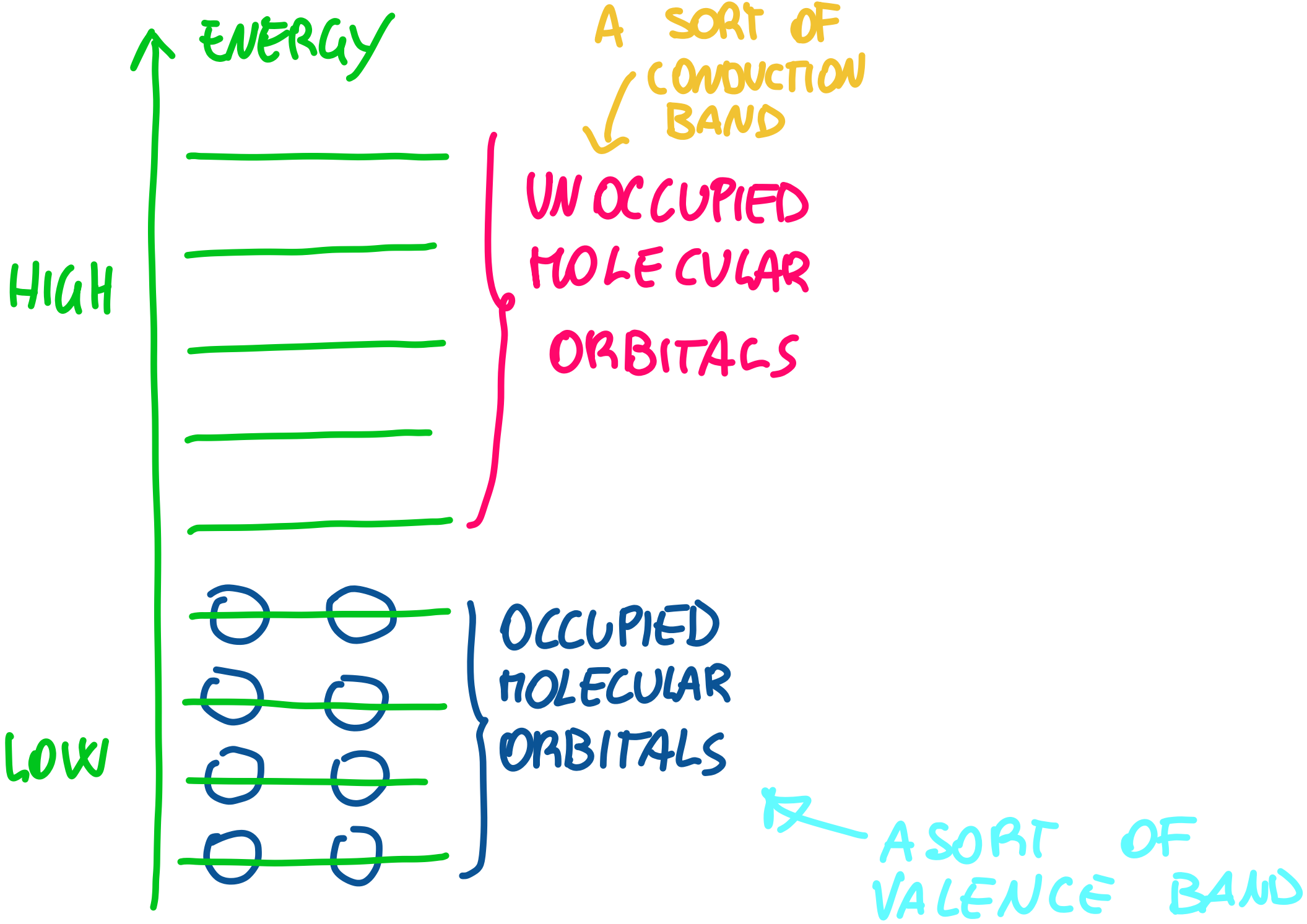
@ ROOM TEMPERATURE

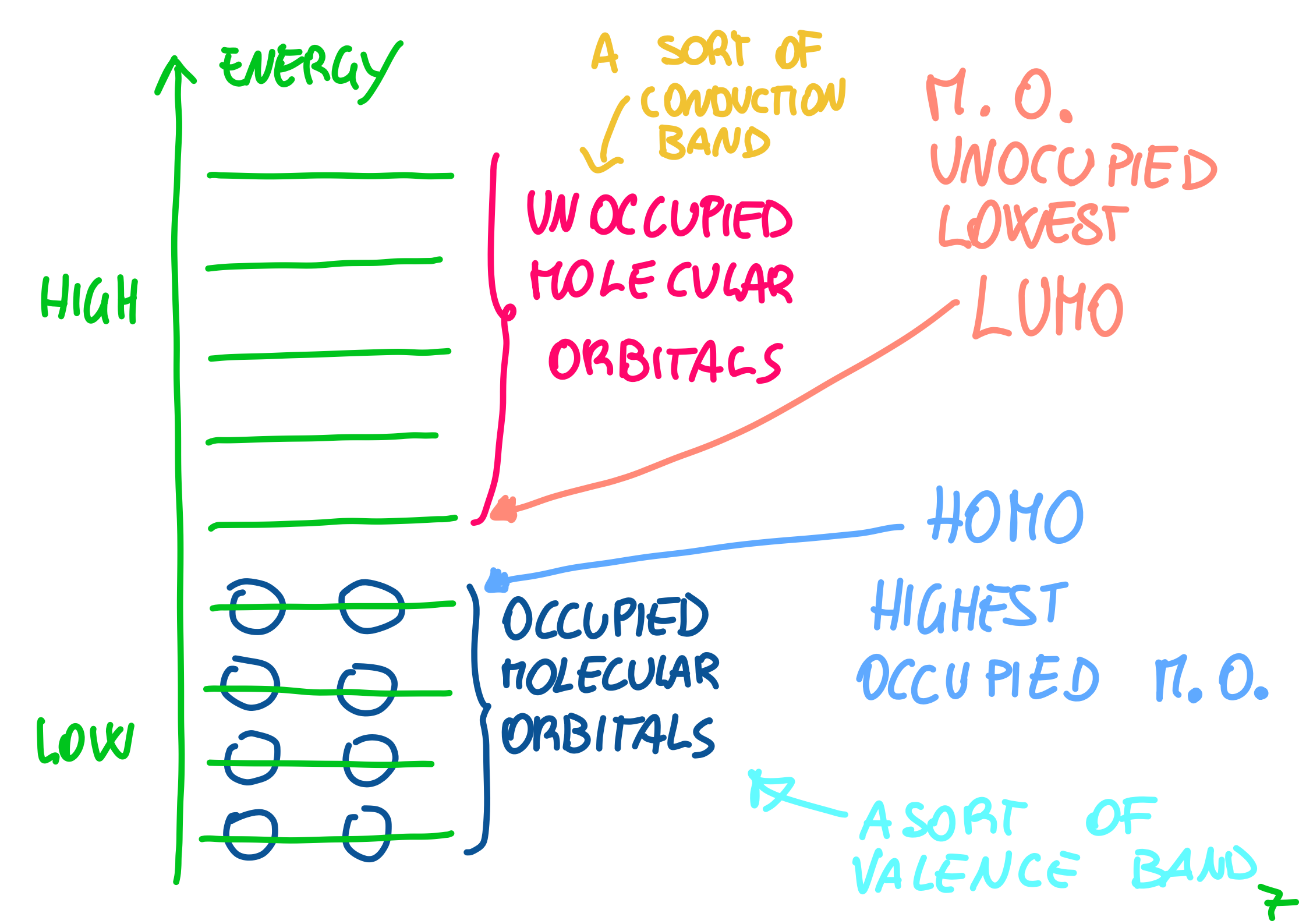
A WAY TO READ MOLECULAR CHARACTERISTICS COMES FROM LCAO

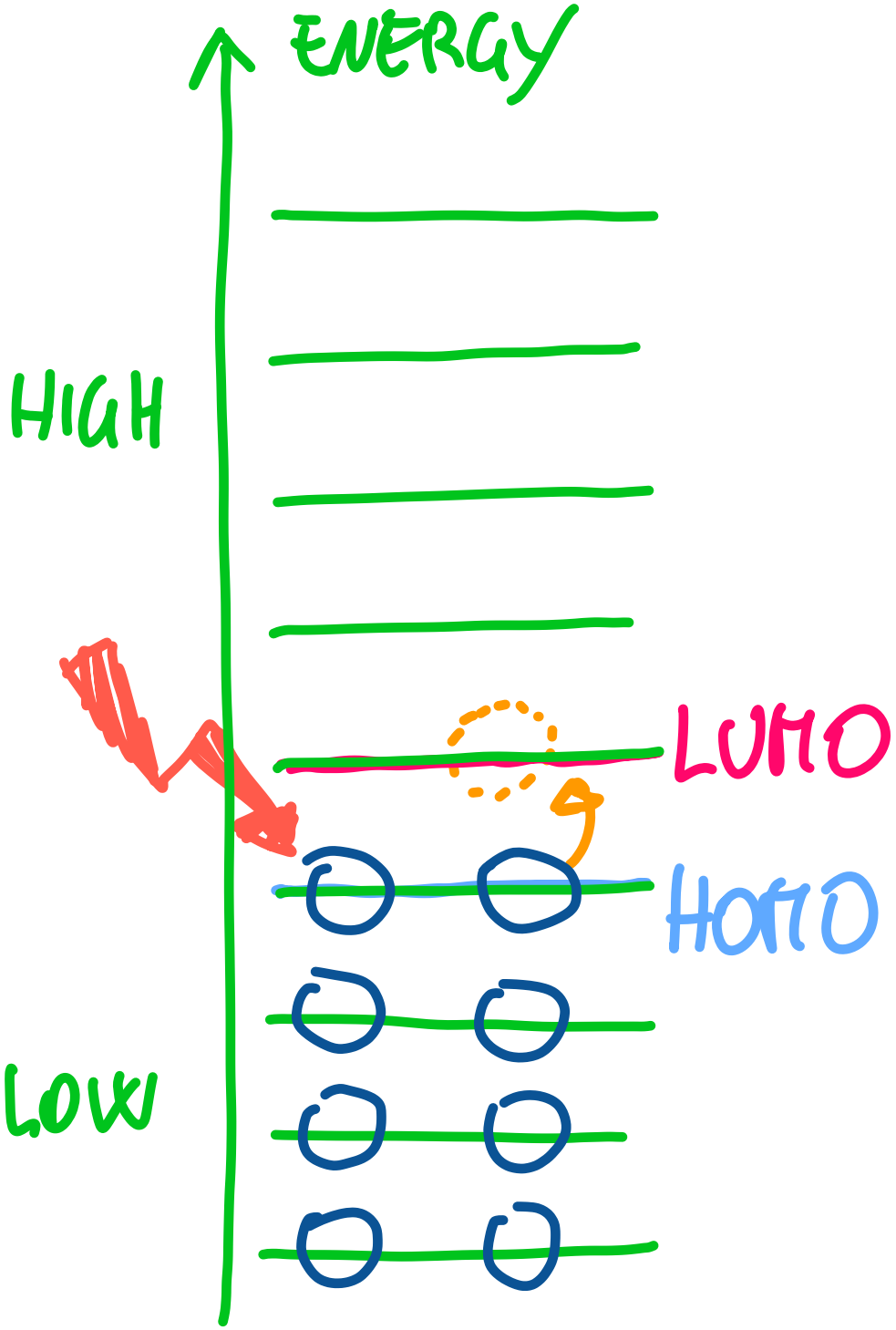
THEORY

LINEAR COMBINATON OF ATOMIC ORBITALS

SOME HINTS IN THE APPENDIX OF. LECTURE NOTES

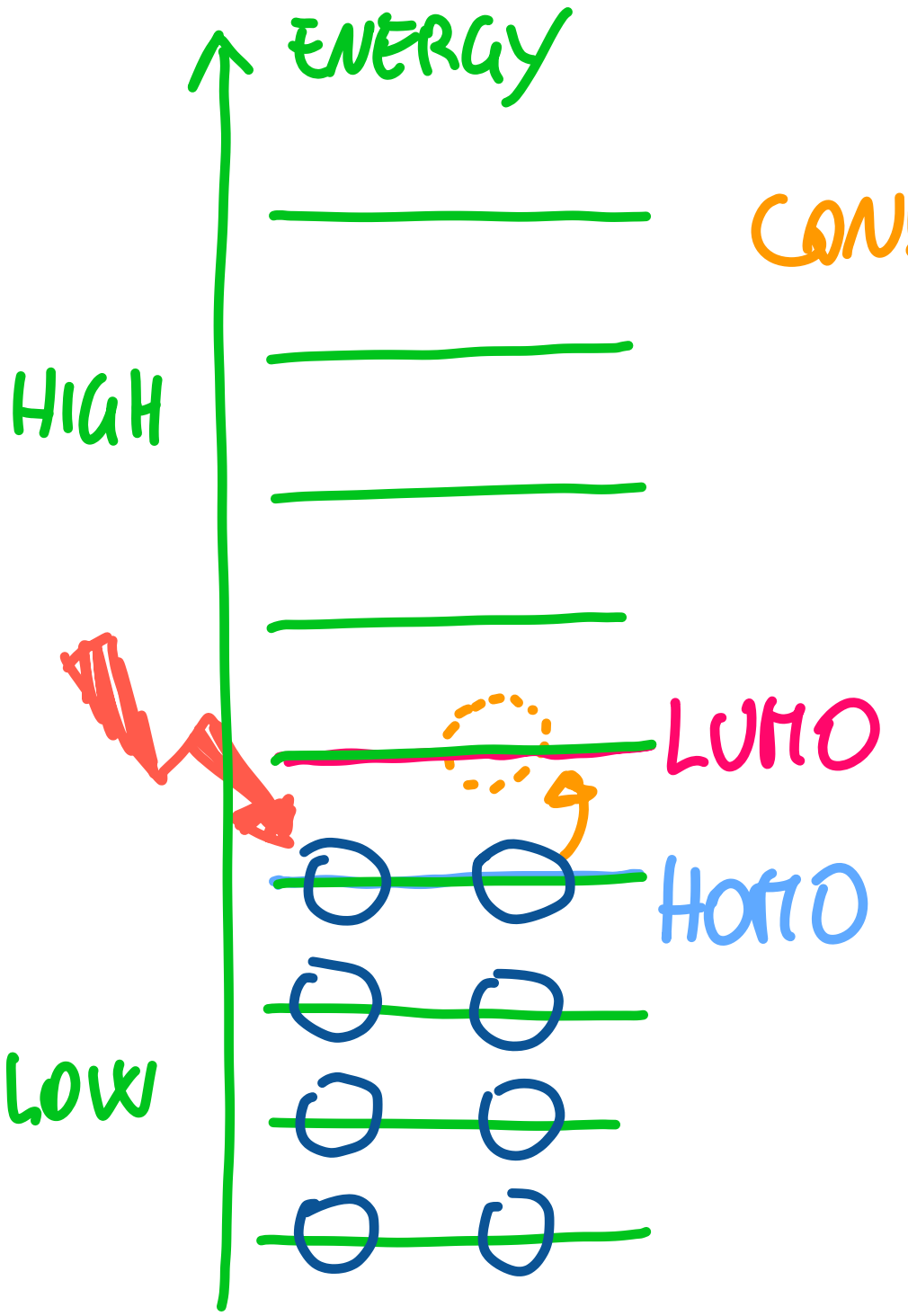

ENERGY
A SORT OF CONDUCTION BAND
UNOCCUPIED MOLECULAR ORBITALS
HIGH
LOW
OCCUPIED MOLECULAR ORBITALS
A SORT OF VALENCE BAND


ENERGY
HIGH
LOW
A SORT OF CONDUCTION BAND
UNOCCUPIED MOLECULAR ORBITALS
M.O. UNOCCUPIED LOWEST
LUMO
HOMO
HIGHEST OCCUPIED M.O.
OCCUPIED MOLECULAR ORBITALS
A SORT OF VALENCE BAND



IF AN EXTERNAL ENERGY EXITES THE MOLECUE 1 ELECTRON COULD JUMP FROM HOMO TO LUMO → LUMO

CONDUCTION HAPPENS



QUALIFIES MOLECULE CONDUCTION SUITABILITY

H L G

↓

HOMO-LUMO GAP

THE SMALLER THE BETTER

H.C.

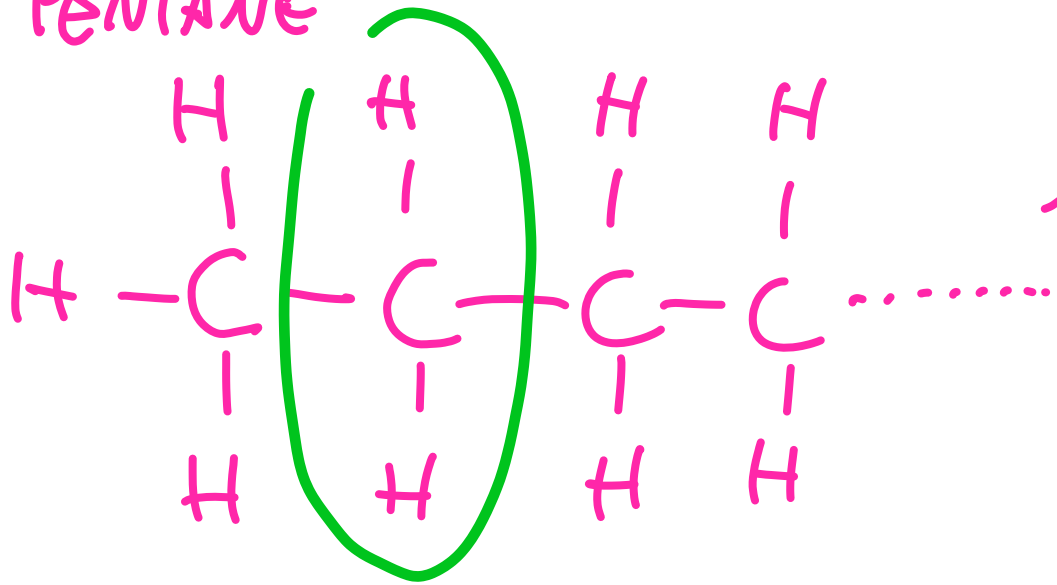
SATURATED / UNSATURATED

↓

ALKANE

- OPEN CHAINS
- MAXMIZE THE N. OF BONDS WITH H FOR EACH C ATOM

EX. PENTANE



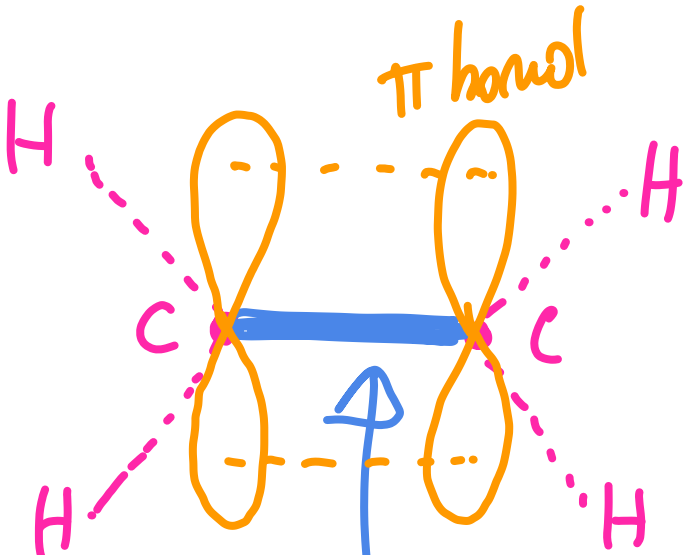
HLG 8eV

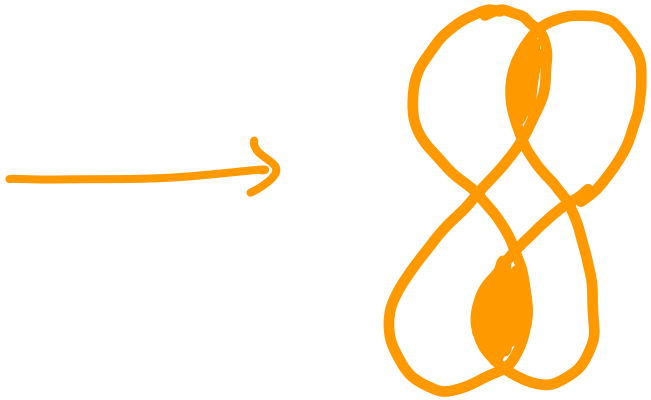
CONSIDERED POOR CONDUCTORS

UNSATURATED HC. DOUBLE OR TRIPLE BOND BW CARBON ATOMS

→ ALKENES → DOUBLE BONDS

ex. ETHENE C_2H_4 $CH_2=CH_2$



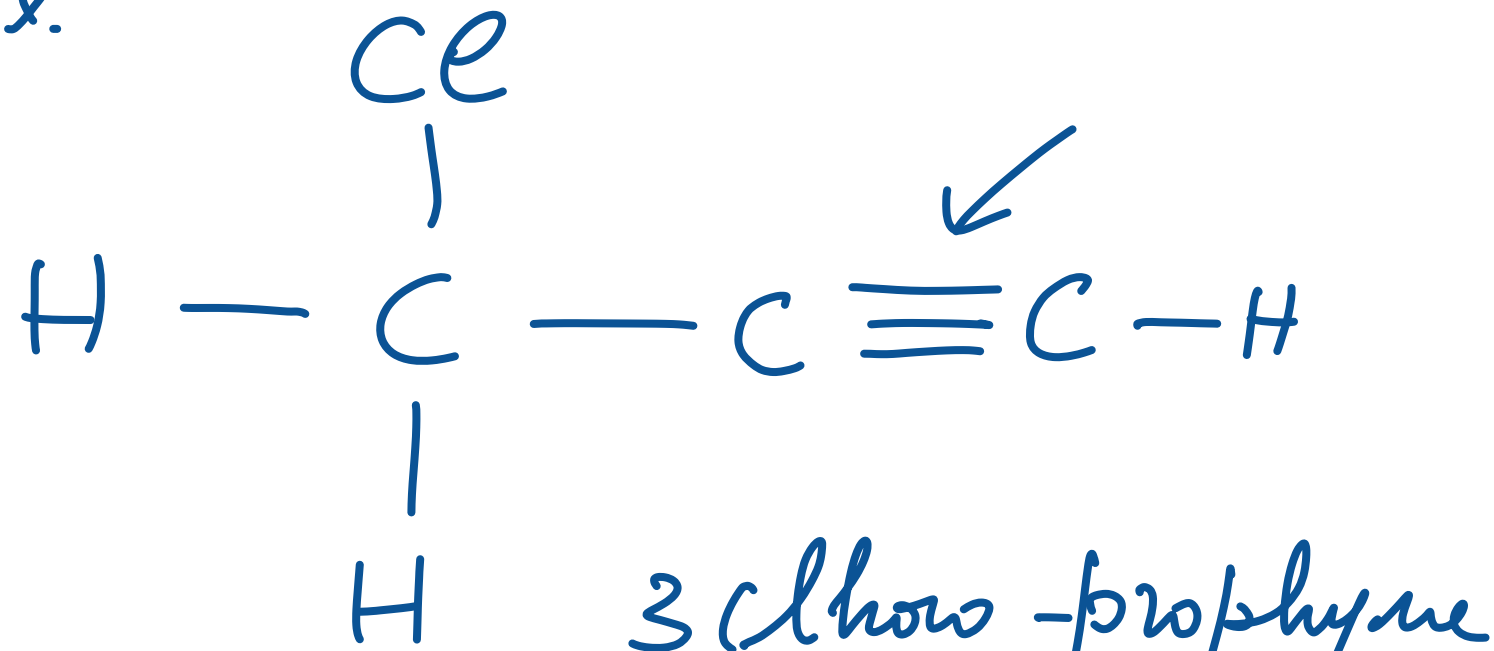


SMALLER HLG

ALKYNE

3 bonds σ et C.

ex.

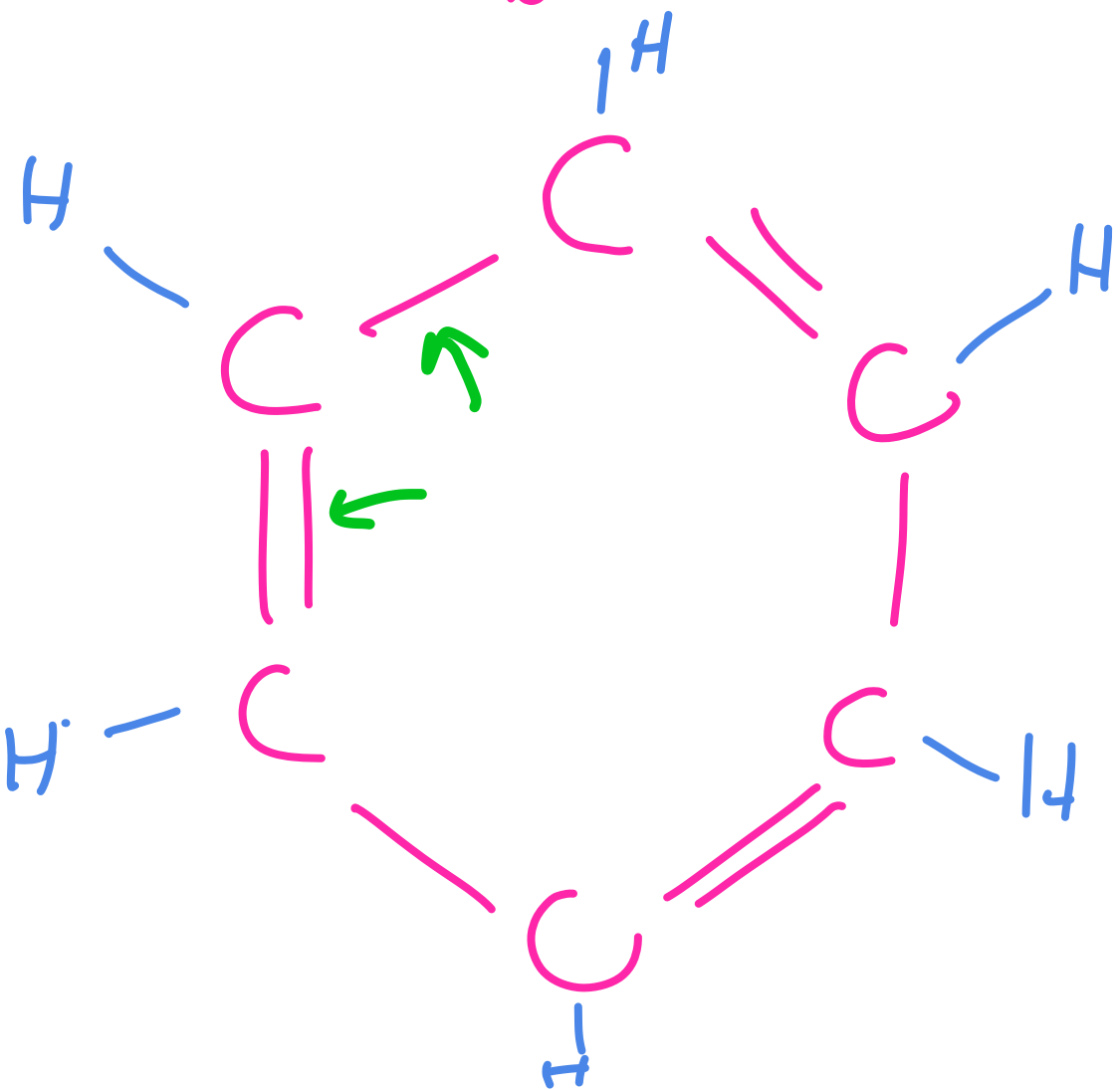


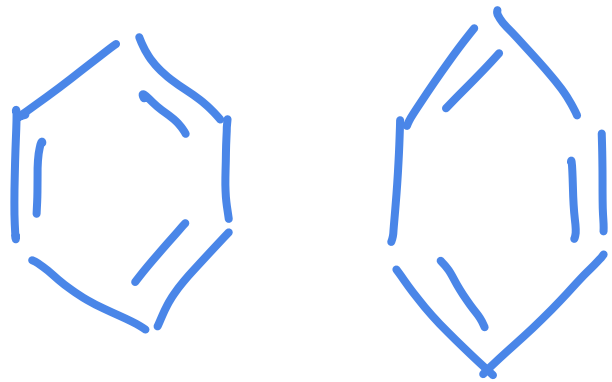
3 chloro-propyne

CYCLIC STRUCTURES

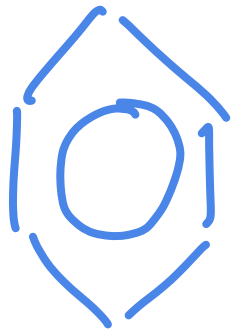
- AROMATIC H.C. AT LEAST 1 RING + OTHER SINGLE OR DOUBLE BONDS

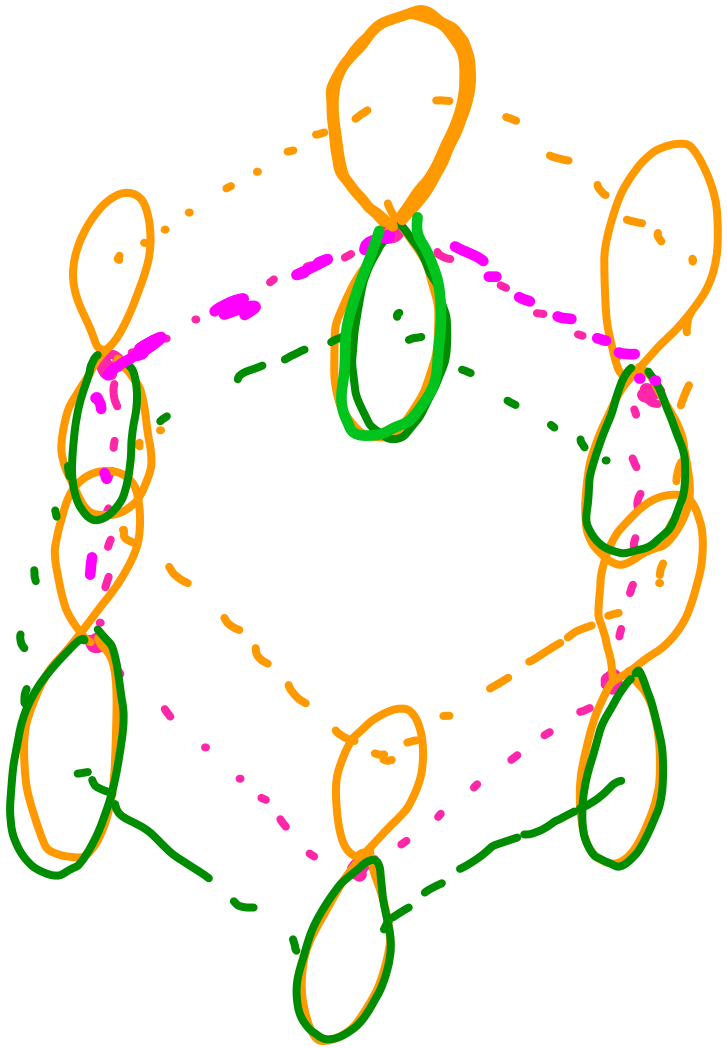
BENZENE C_6H_6

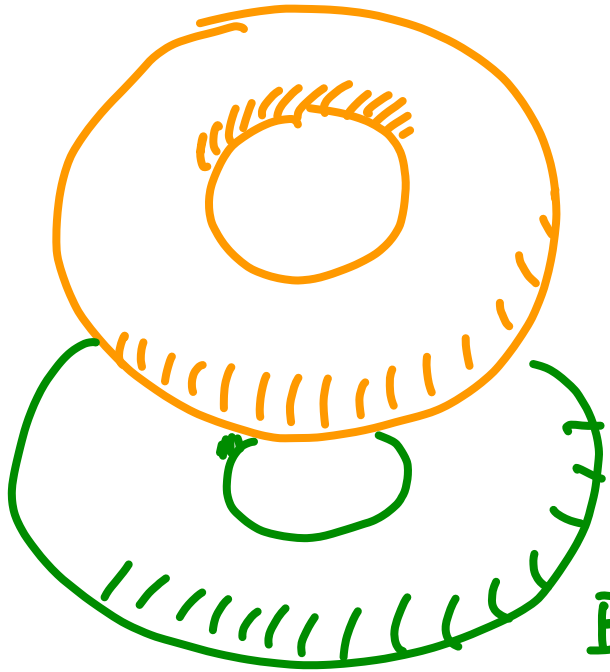




RESONANT MOLECULES







TOP RING

BOTTOM RING

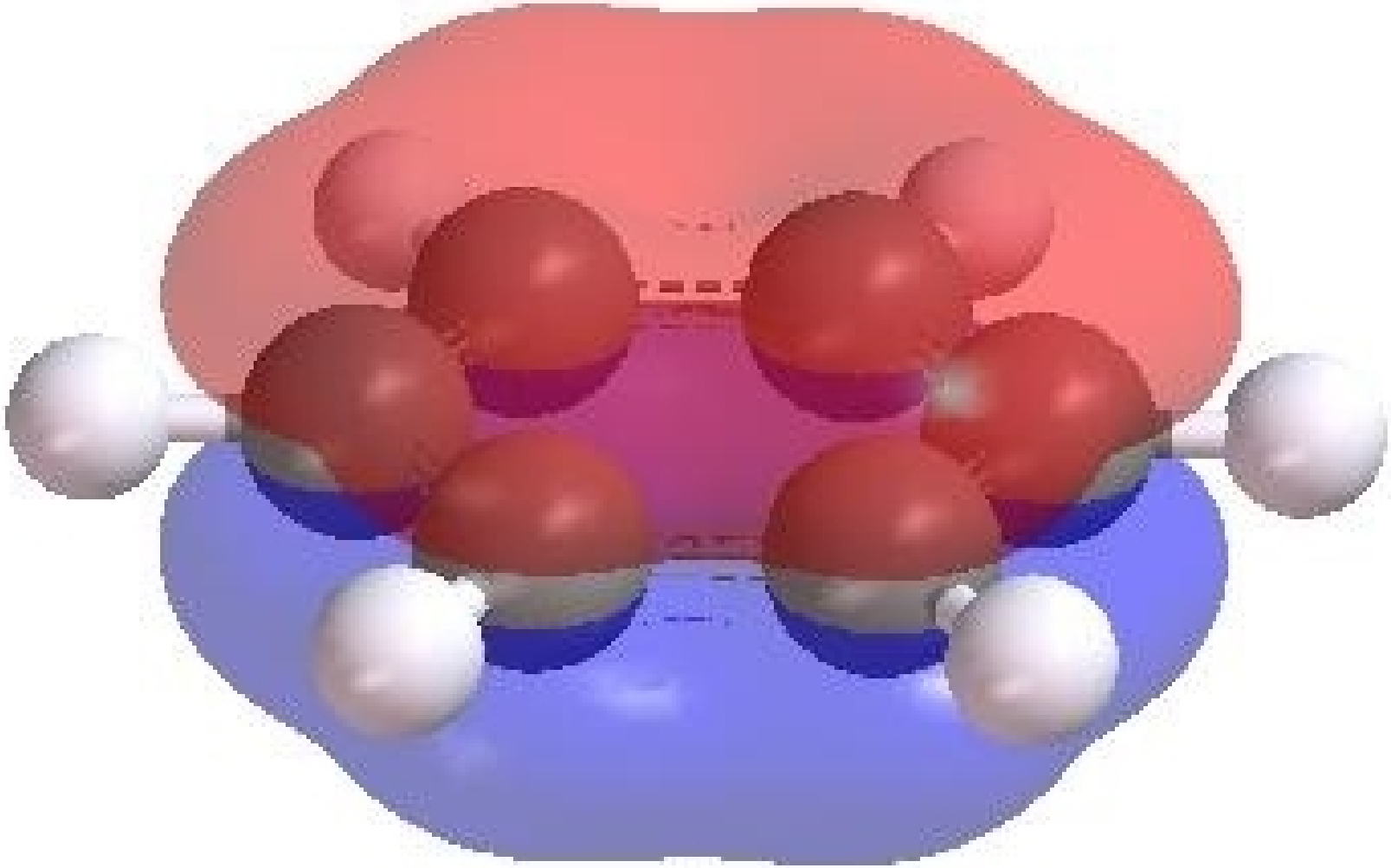
ELECTRONS ARE DELOCALIZED IN A UNIQUE CLOUD

↓

VERY GOOD PROP. FOR CONDUCTION

(AVOGADRO)

ANOTHER VIEW OF THE 2 RINGS



SAID CONJUGATED MOLECULE IS

...AND THIS IS ANOTHER ONE.....

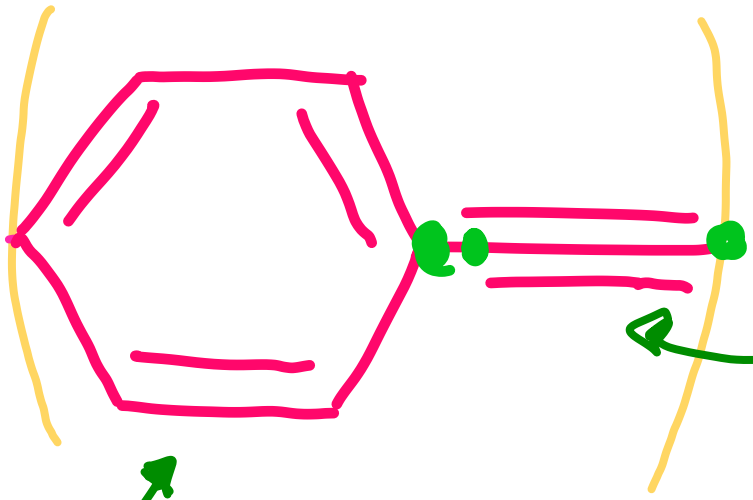
SOME OF THE MOLECULES USED FOR MOLECULAR TRANSISTOR

(SO MANY IN THE SCIENTIFIC LITERATURE!)

BASED ON BENZENE

OPE OPV OT PCP

OPE OLIGO PHENYLEN ETHYNYLENE



ETHYNYLENE

$-C\equiv C-$

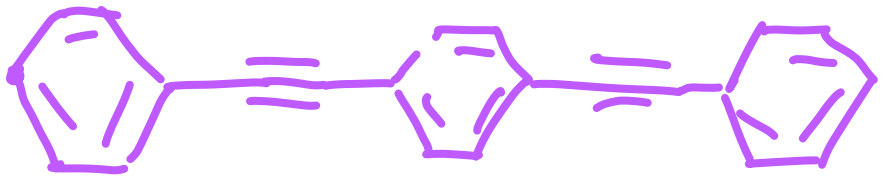
PHENYLENE

(BENZENE WITHOUT 1 O 2 H

PHENYL

ACETYLENE $H-C\equiv C-H$

ex CHAIN OF 3 OPE ELECTRONS DELOCALIZED

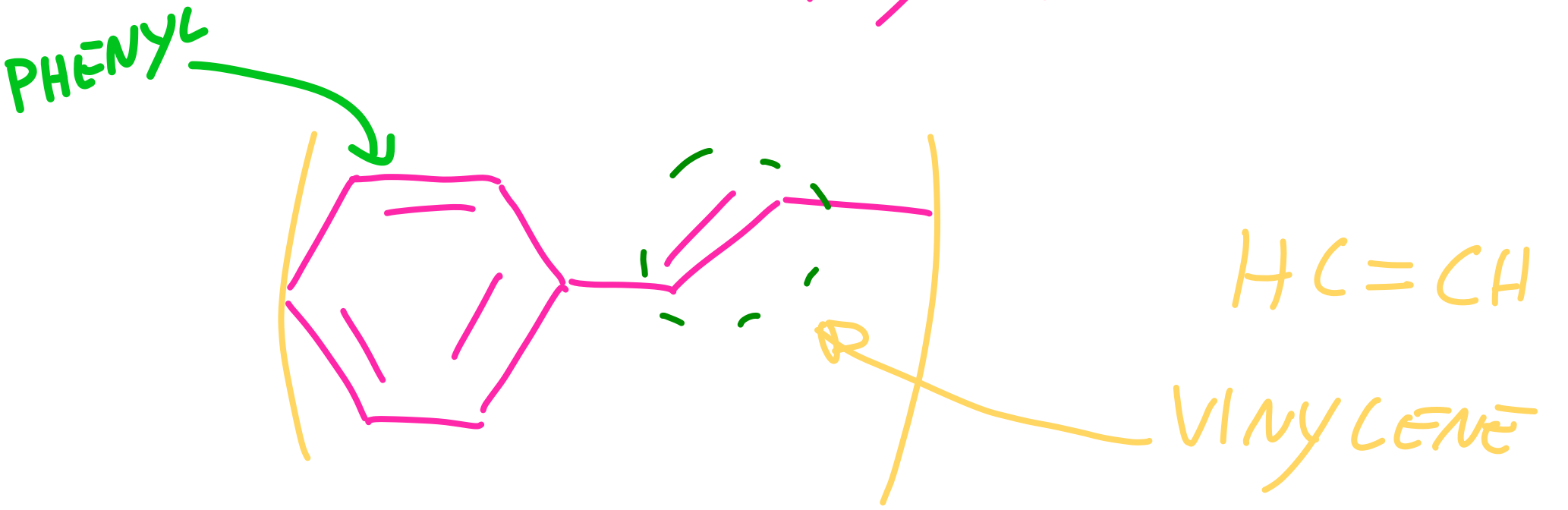


HLG 3.5 eV

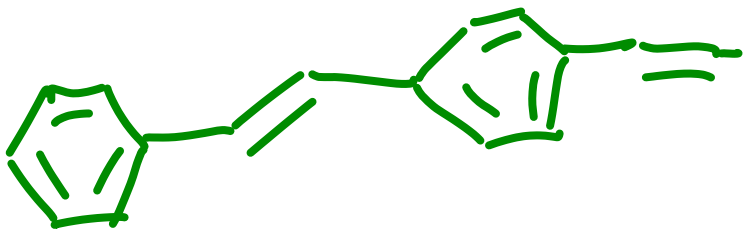
OPE

- EASY TO GENERATE LONG CHAINS → FORO EC., BIG CURRENT
- SUBJECT TO TORSION → CURRENT REDUCES

OPV OLIGO PHENILENE VINYLENE

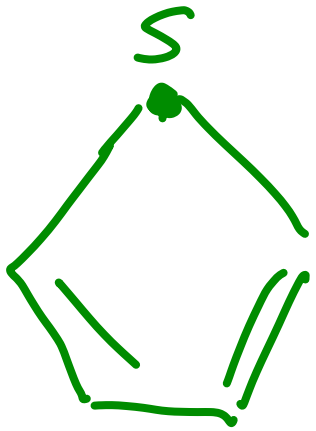


HLG 3.1 eV



TORSION LESS POSSIBLE, MORE PLANAR

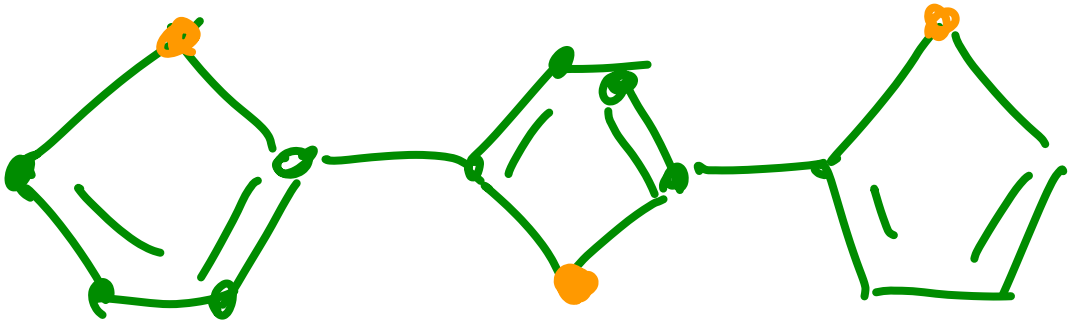
OT OLIGO THIOPHENE



4C 1S (SULFUR)

π bonds in RING

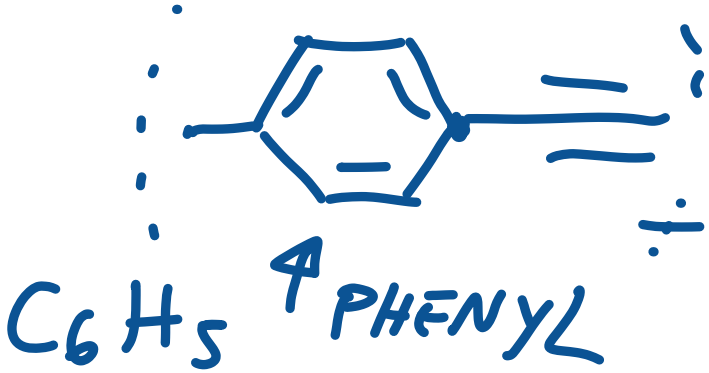
HLG 2.9eV



CASE PCP PARACYCLOPHANE

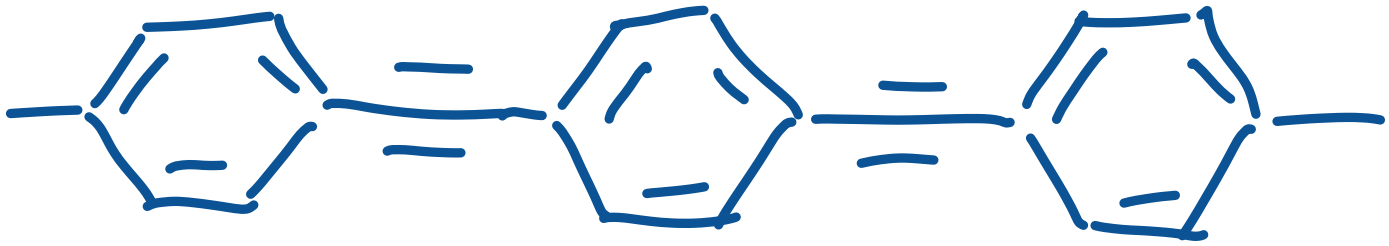
BASED ON OPE

OPE

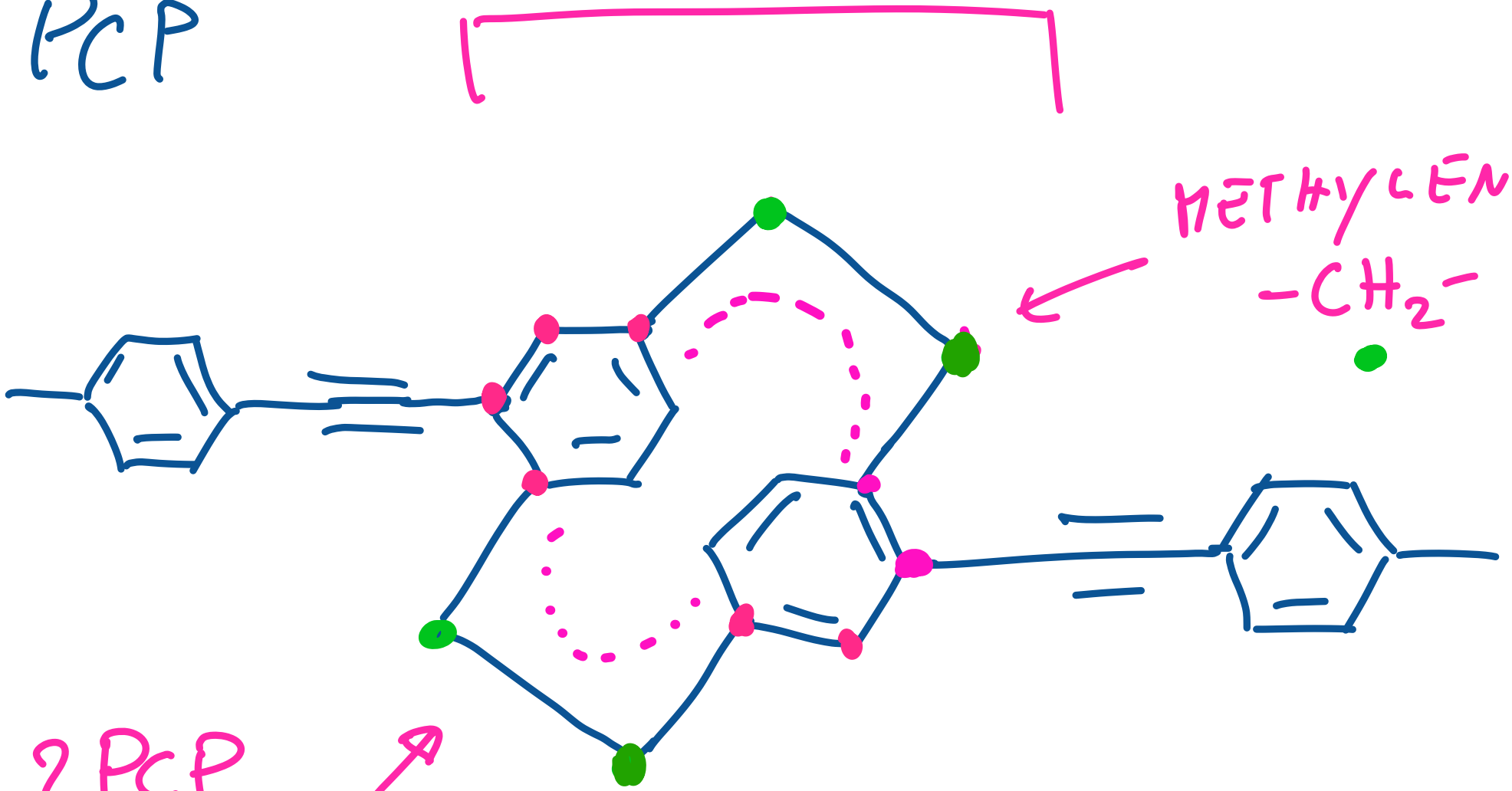


STARTING FROM

OPE3



PCP



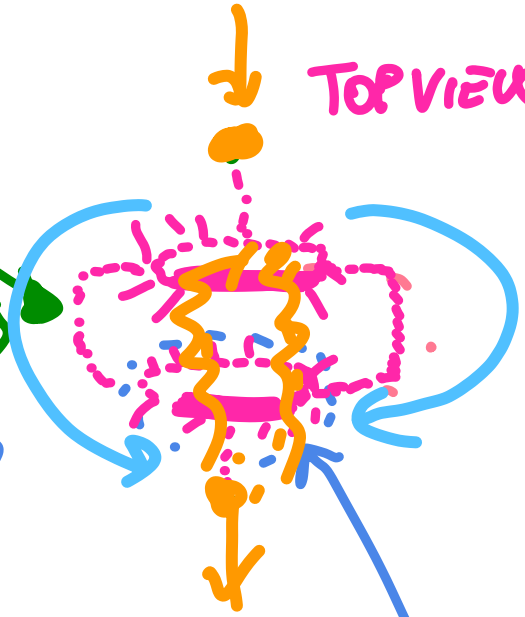
2,2 PCP → BRIDGE WITH A CHAW OF 2 METHYLEN.

3,3 PCP → BRIDGE 3 METH...

2>

2,2 PCP

THE BRIDGE INFLUENCE THE CONJ. SYSTEM

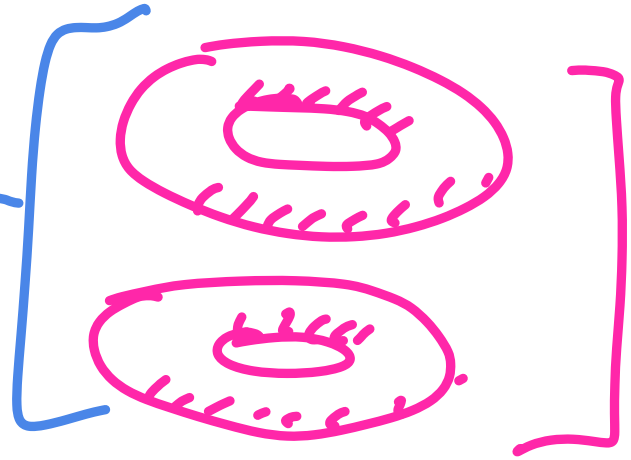


EACH RING IS A CONJUGATED SYSTEM OF

π ORBITALS

2 RINGS FACED:

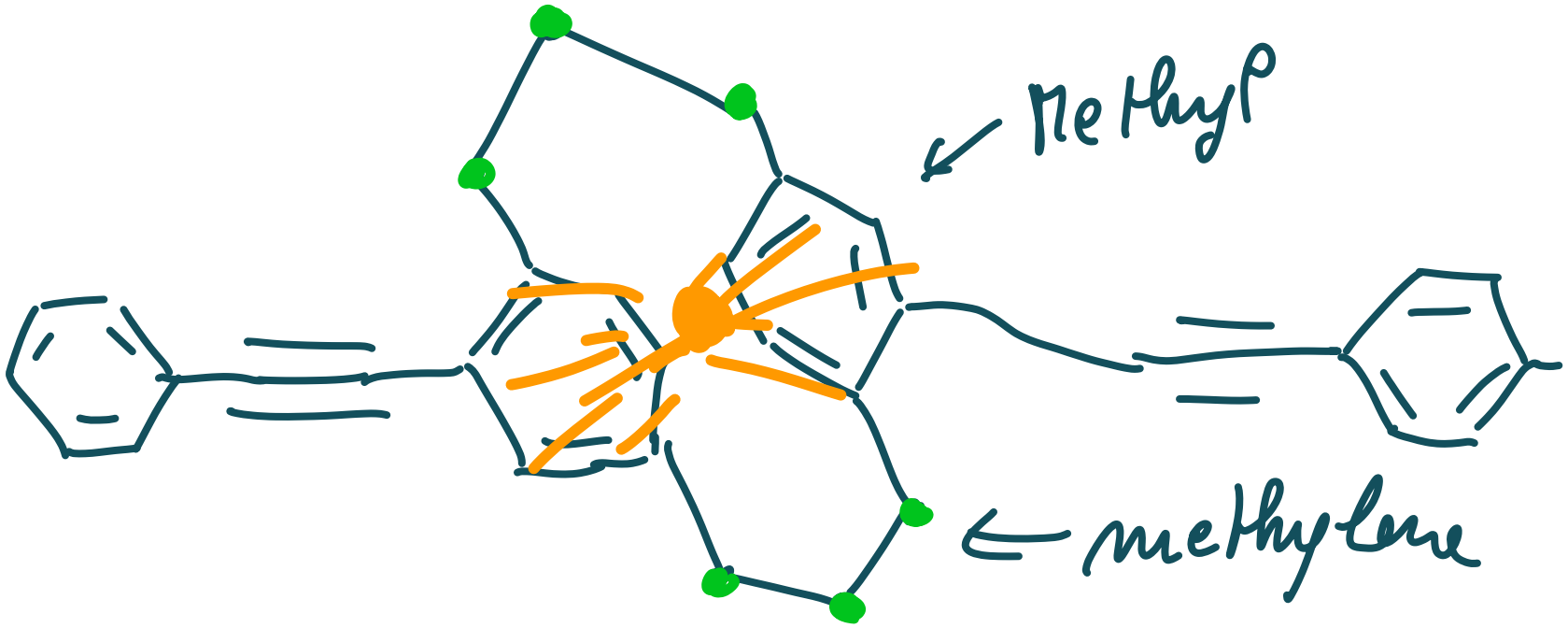
2 FACED CONJ. SYSTEMS



1 RING

3.3 PCP

CYCLOPHANE - BASED M. SEN.



OTHER MOLECULES USED IN THIS COURSE

→ FULLERENE FAMILY

FOR SENSORS
FOR MEMORY

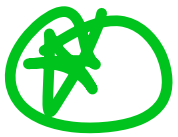
→ BISFERROCENES

FOR FCNN

CRISTALLIZATION :

- HOMO - LUMO & HLG
- CLASSIFICATION : ALKANE - ALKENE
  ALKYNE
  CONJUGATED

POINTER



- SET OF MOLECULES :
  OPE OPV OT PCP