

# COMPUTATIONAL CHEMISTRY DAY 2023

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## Molecular design and computational investigation of optoelectronic properties of conjugated polymers for OPV cells

**PAU** BEARN  
PYRÉNÉES  
Communauté d'Agglomération



**UNIVERSITÉ**  
DE PAU ET DES  
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**cnrs**



# Materials for OPV cells

Renewable energies

Sources (most available)

Materials (pollution/cost)

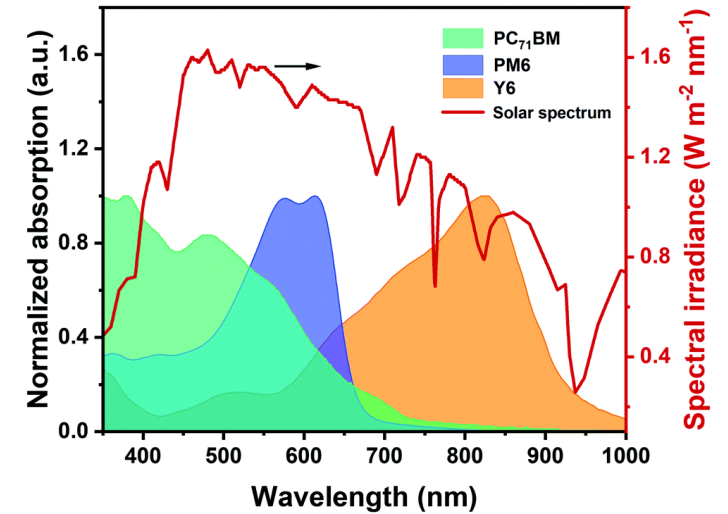
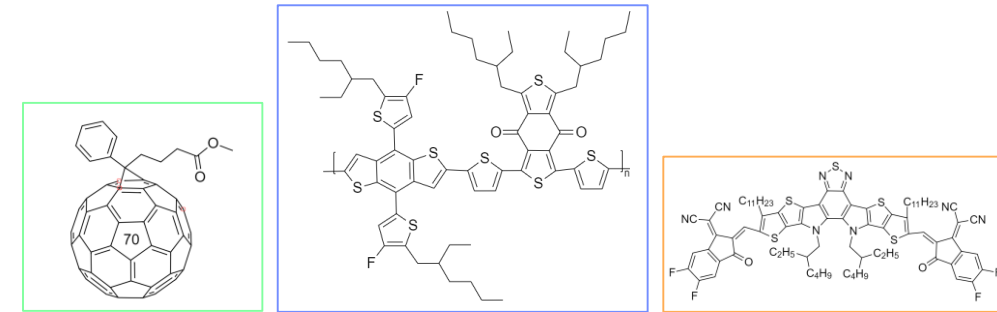
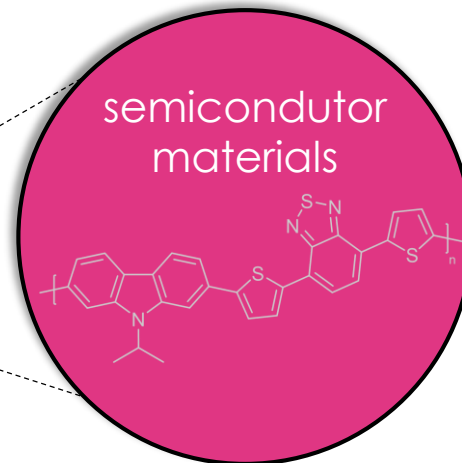
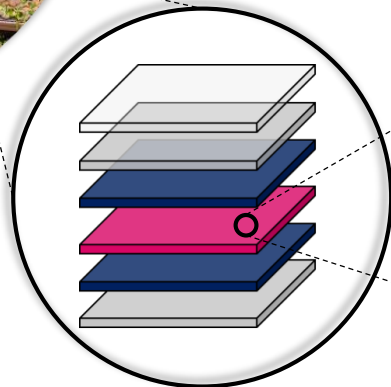
Photovoltaic technologies

Organic devices

Lighter weight

Mechanical flexibility

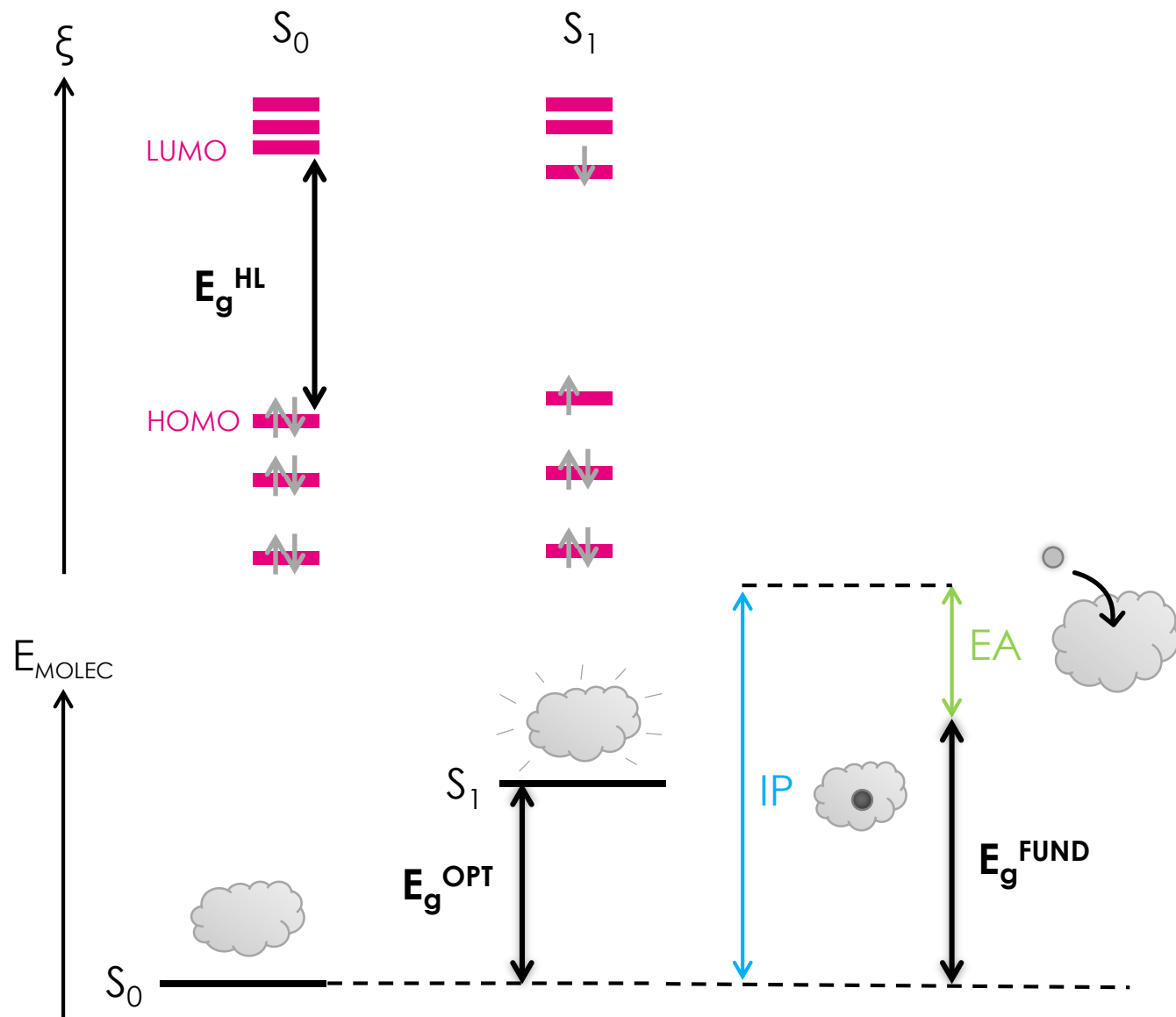
Recyclable



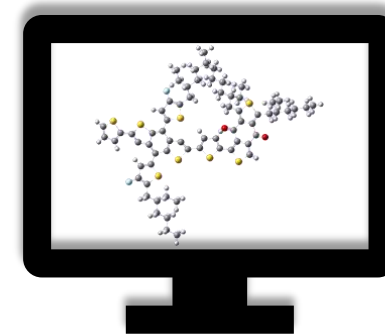
*Mater. Chem. Front.*, 2020, **4**, 3487-3504

Light absorption ↔ material

$E_g$

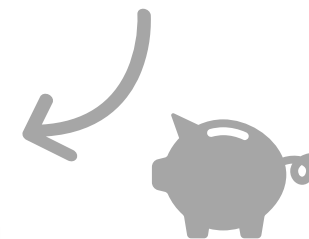


Model molecules  
+  
Estimate properties



New materials

Polymer structure

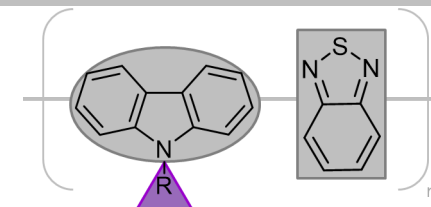
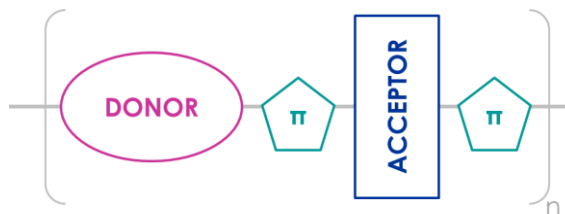
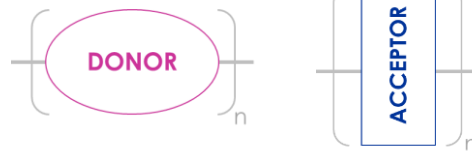
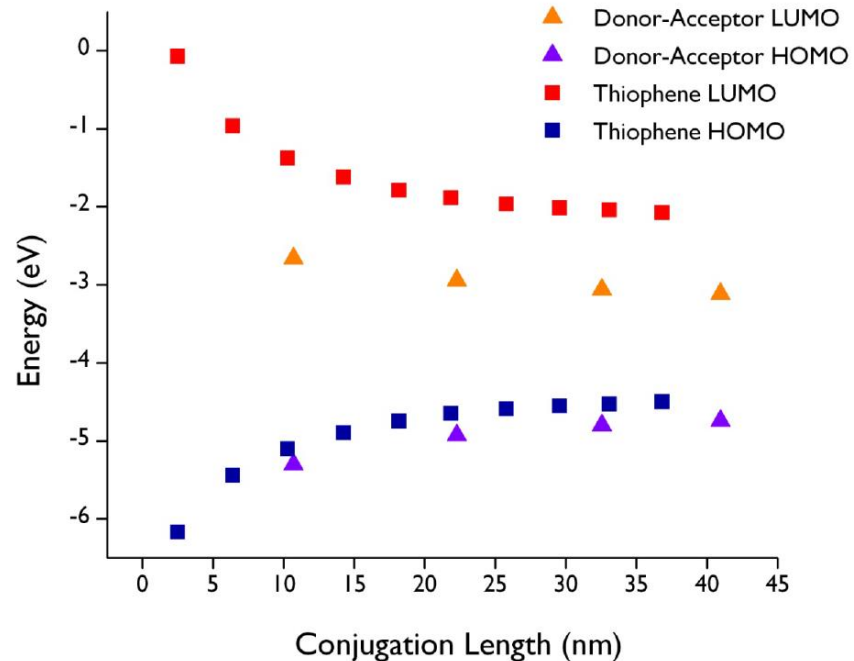
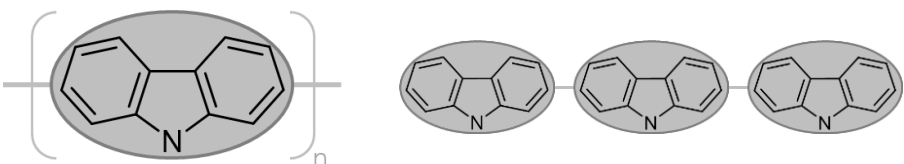


# Molecular design of conjugated polymers

## Conjugation length

## Nature of blocks

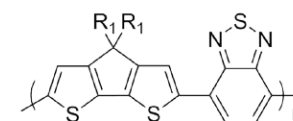
## Side chains



$$E_g^{\text{OPT}} [\text{eV}]$$

B3LYP / 6-311G(d)

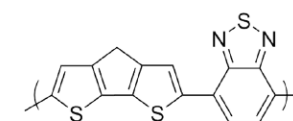
1.36



PCPDTBT

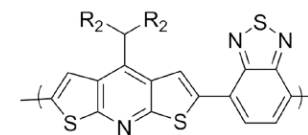
R<sub>1</sub> = 2-ethylhexyl

1.39



PCPDTBT-H

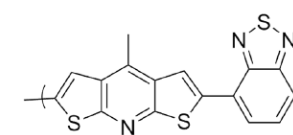
2.05



PDTpN-BT

R<sub>2</sub> = n-octyl

2.07



PDTpN-BT-H

Figure S1. Energy level of the LUMO and HOMO plotted as a function of conjugation length for 3-methylthiophene oligomers and oligomers of compound 17.

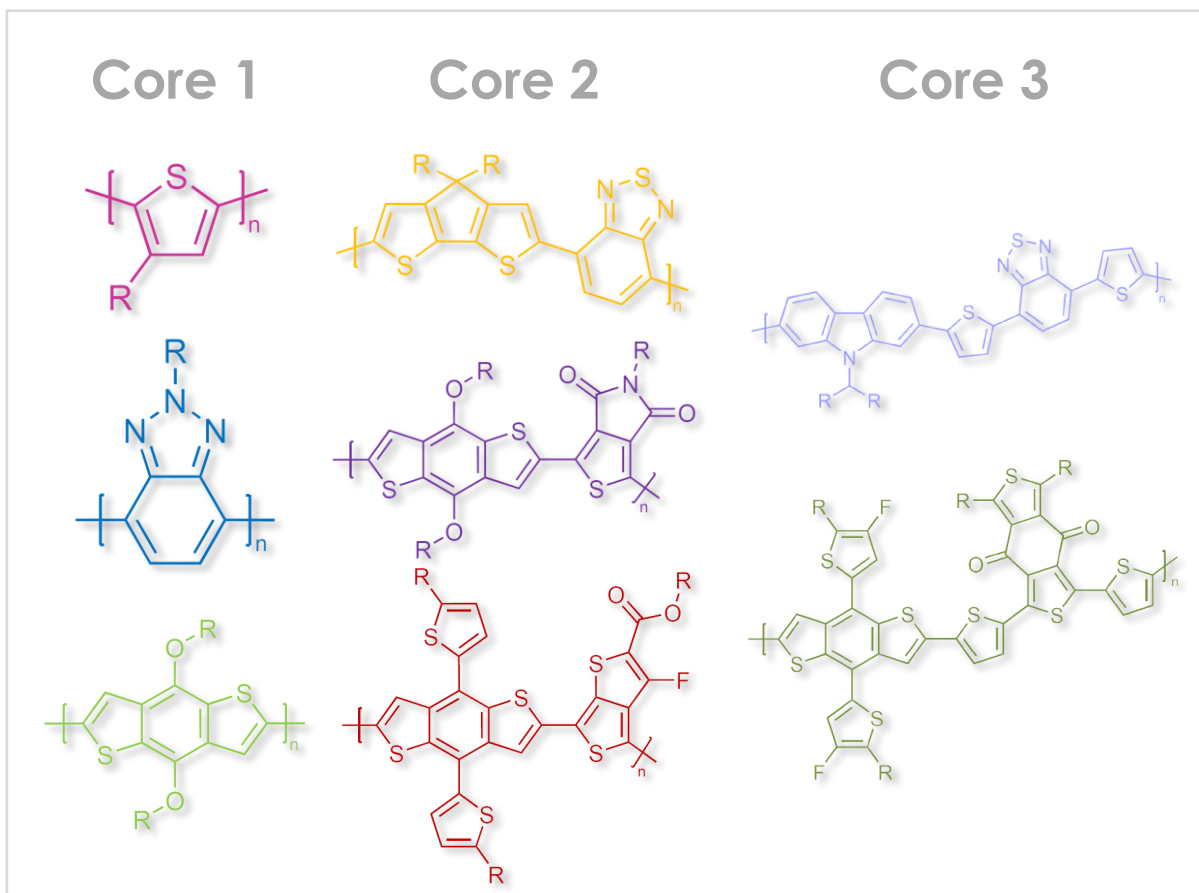
# This work

Conjugation length

Nature of blocks

Side chains

Double chains



$E_g^{HL}$	$S_0$ : HOMO-LUMO	DFT
$E_g^{OPT}$	$E_{S_1} - E_{S_0}$ (vertical transition)	TD-DFT
$E_g^{FUND}$	IP – EA IP: $E_+ - E_0$ EA: $E_- - E_0$	DFT



B3LYP  
6-31G(d)  
D3 correction

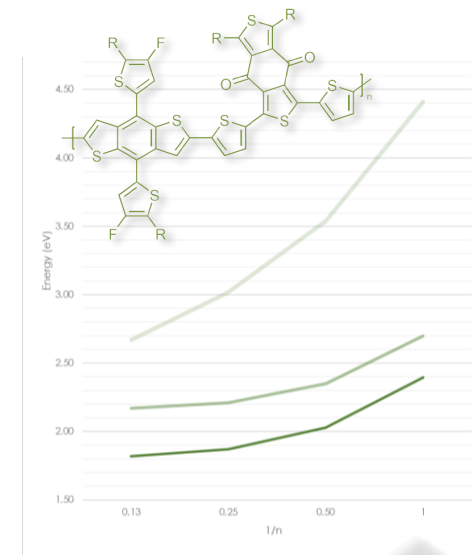
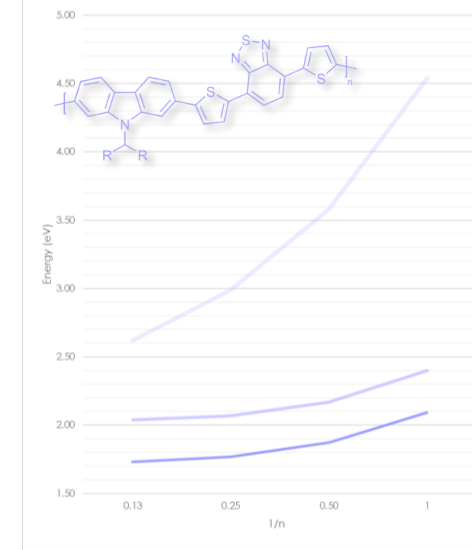
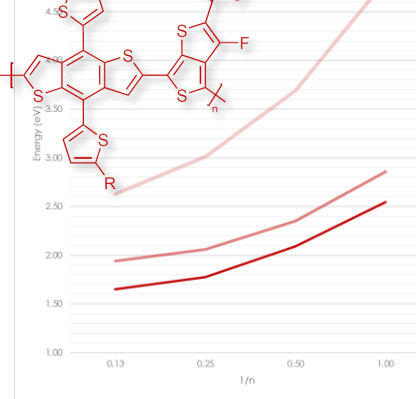
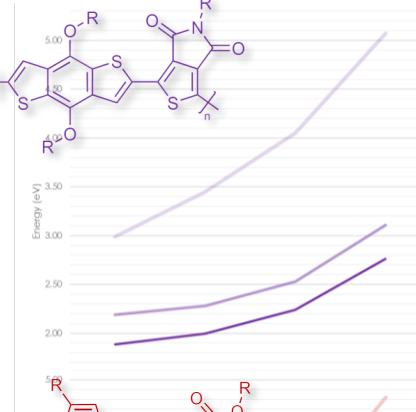
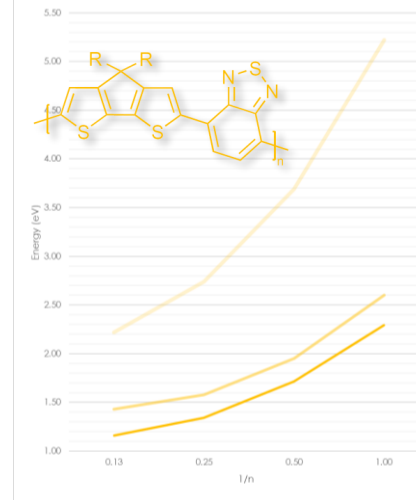
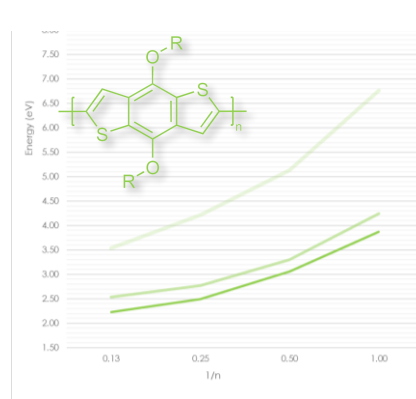
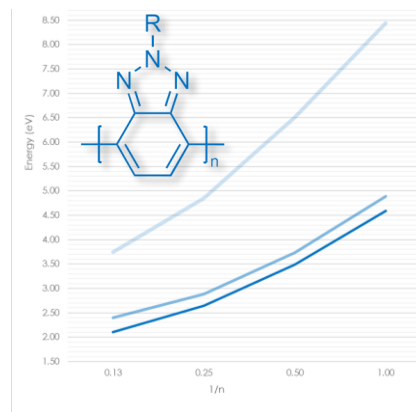
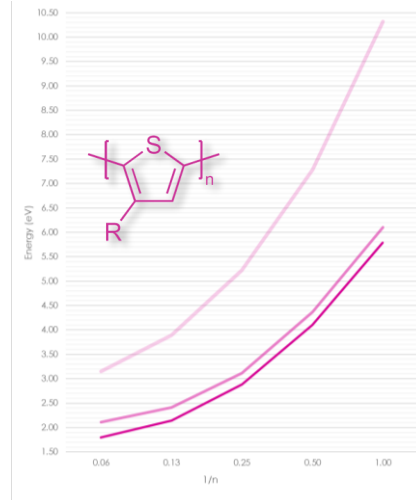
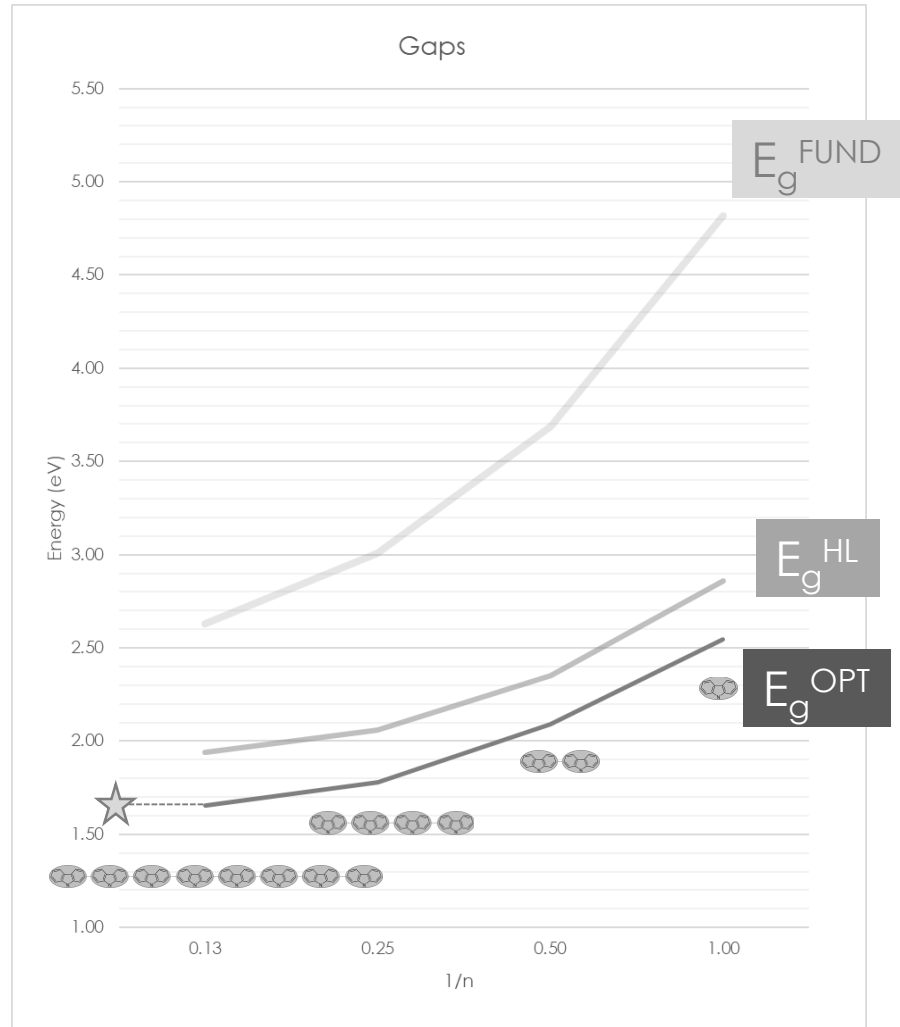
Total CPU time: ~2.000.000 h

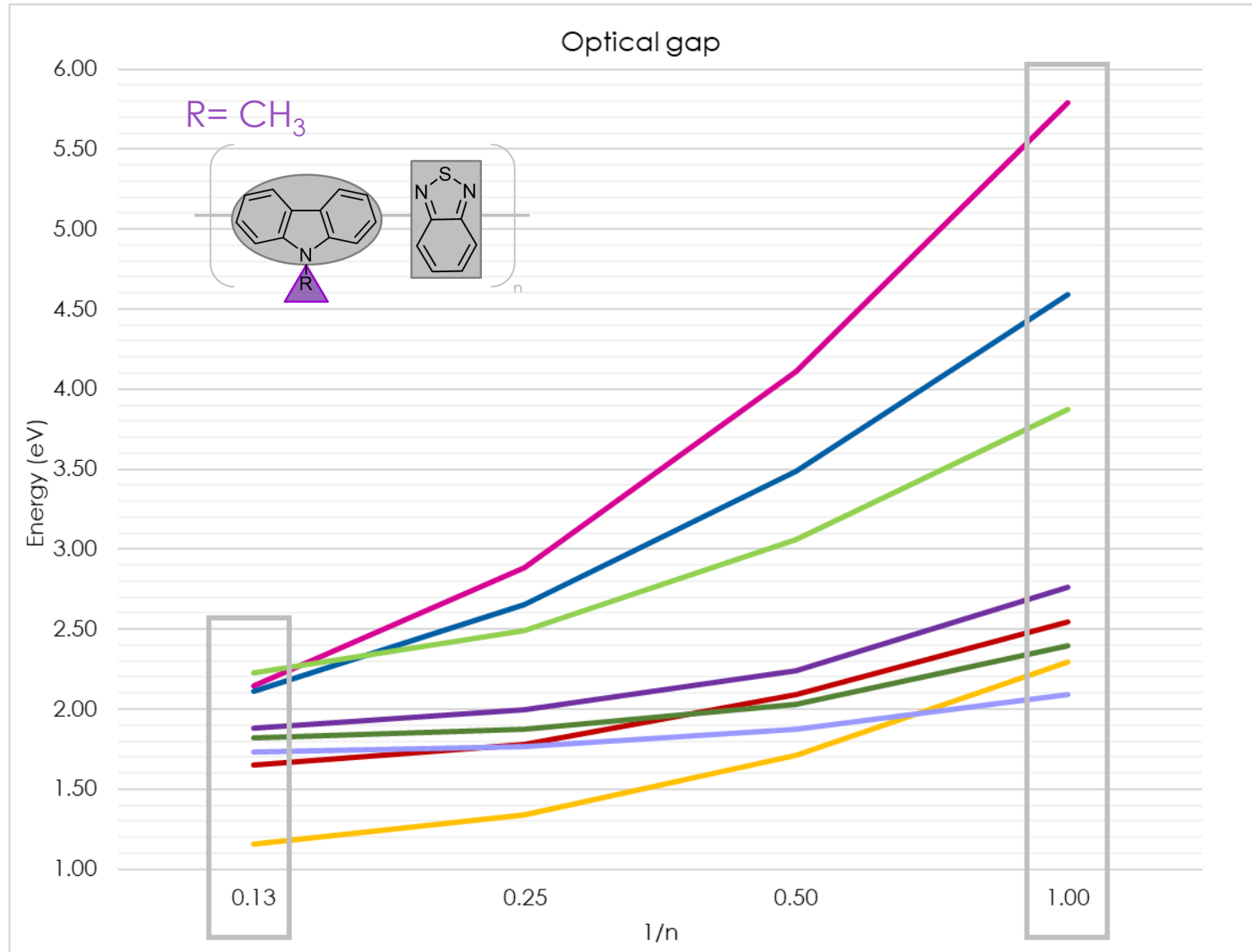
# Conjugation length

# Nature of blocks

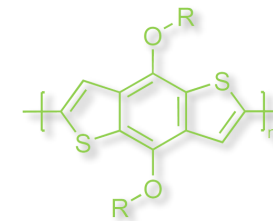
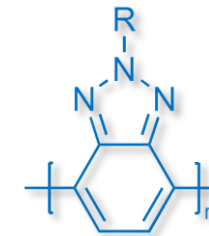
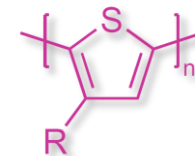
# Side chains

# Double chains

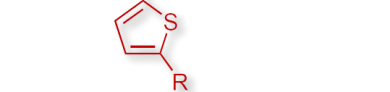
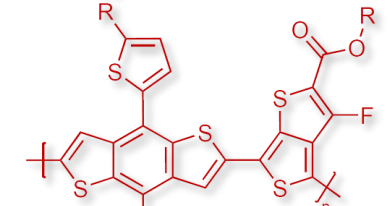
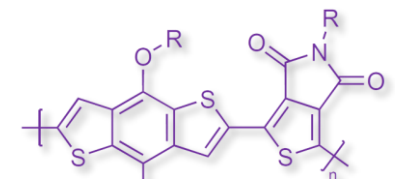
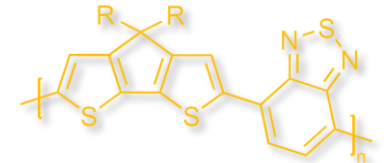




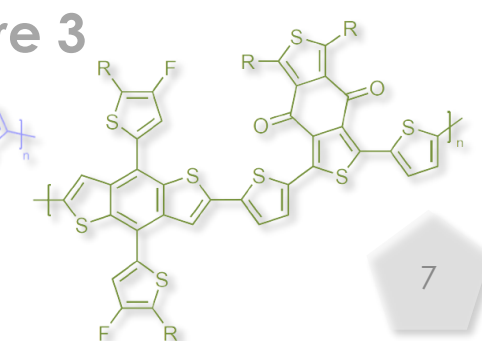
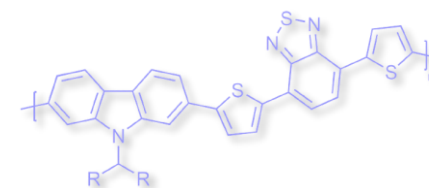
Core 1



Core 2



Core 3

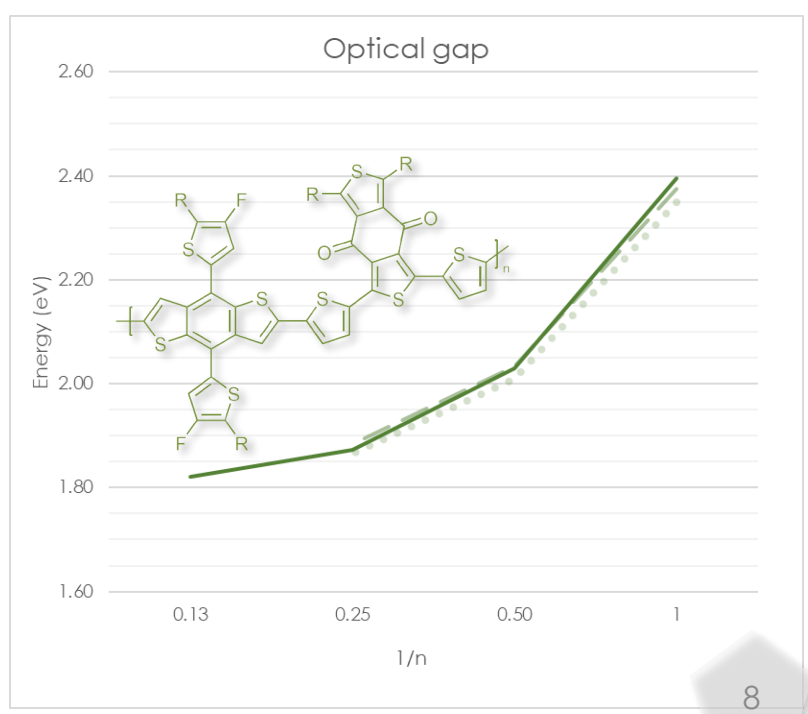
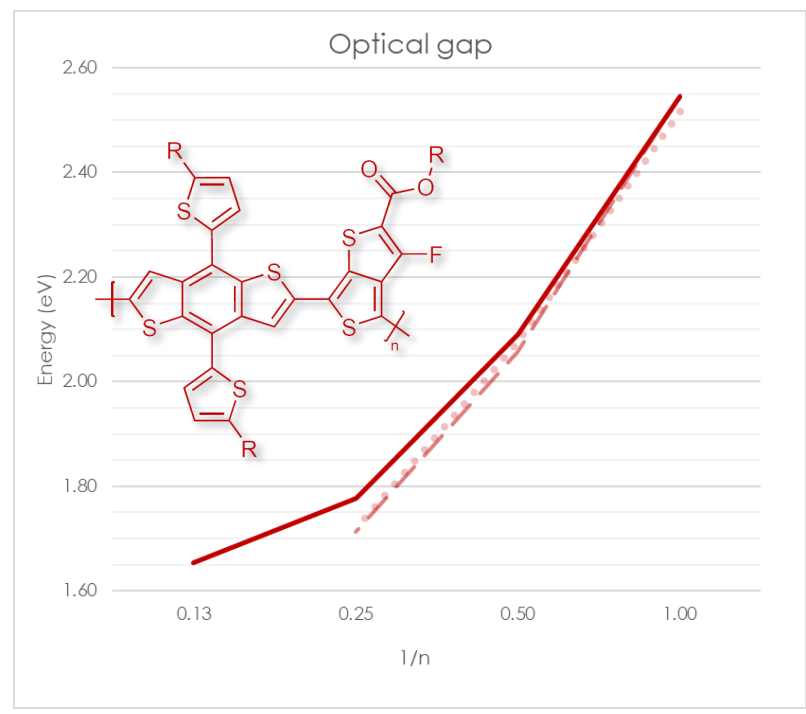
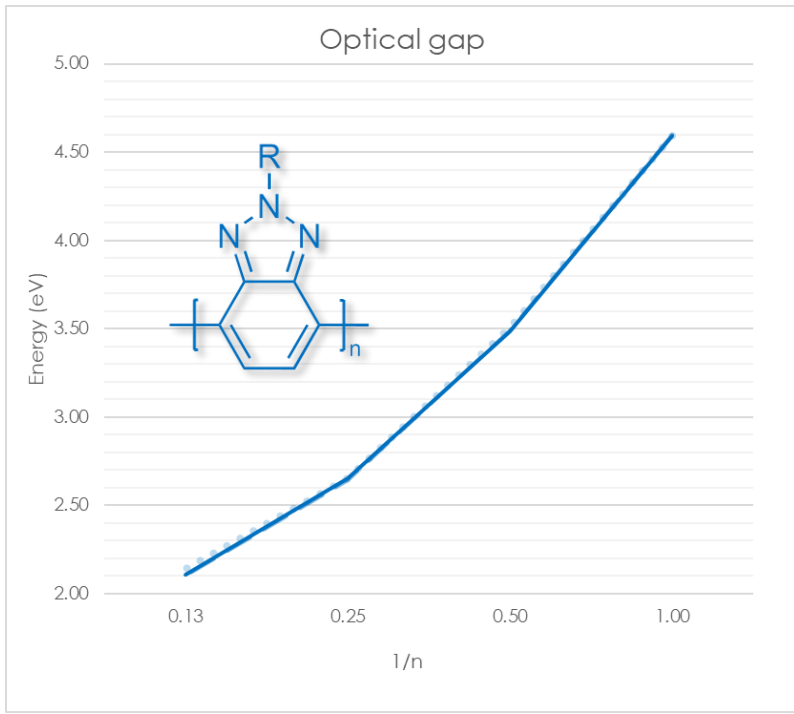
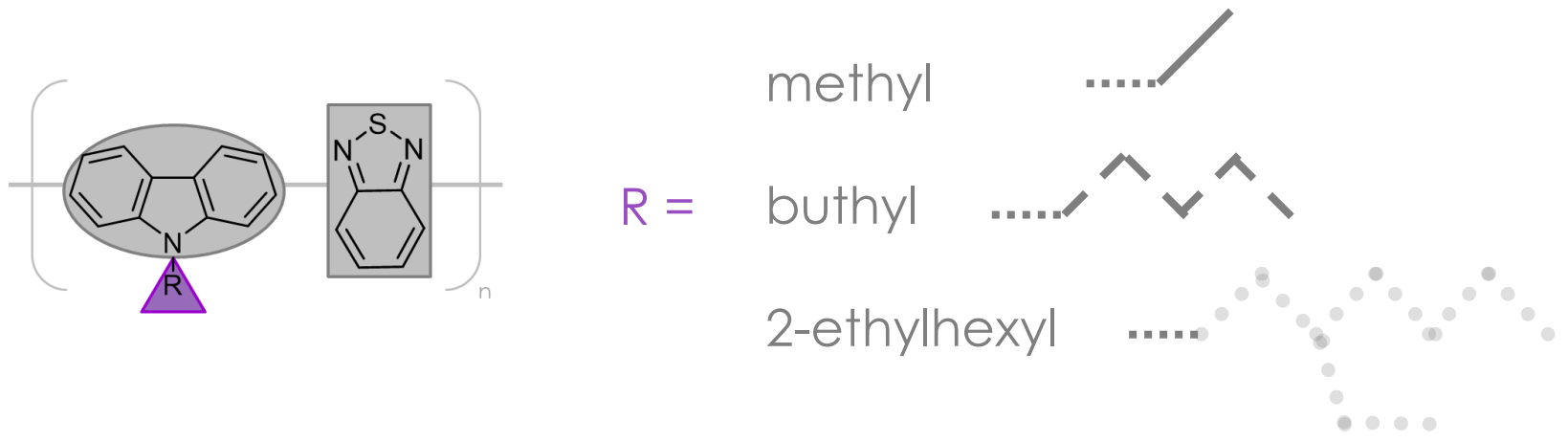


# Conjugation length

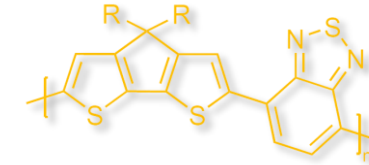
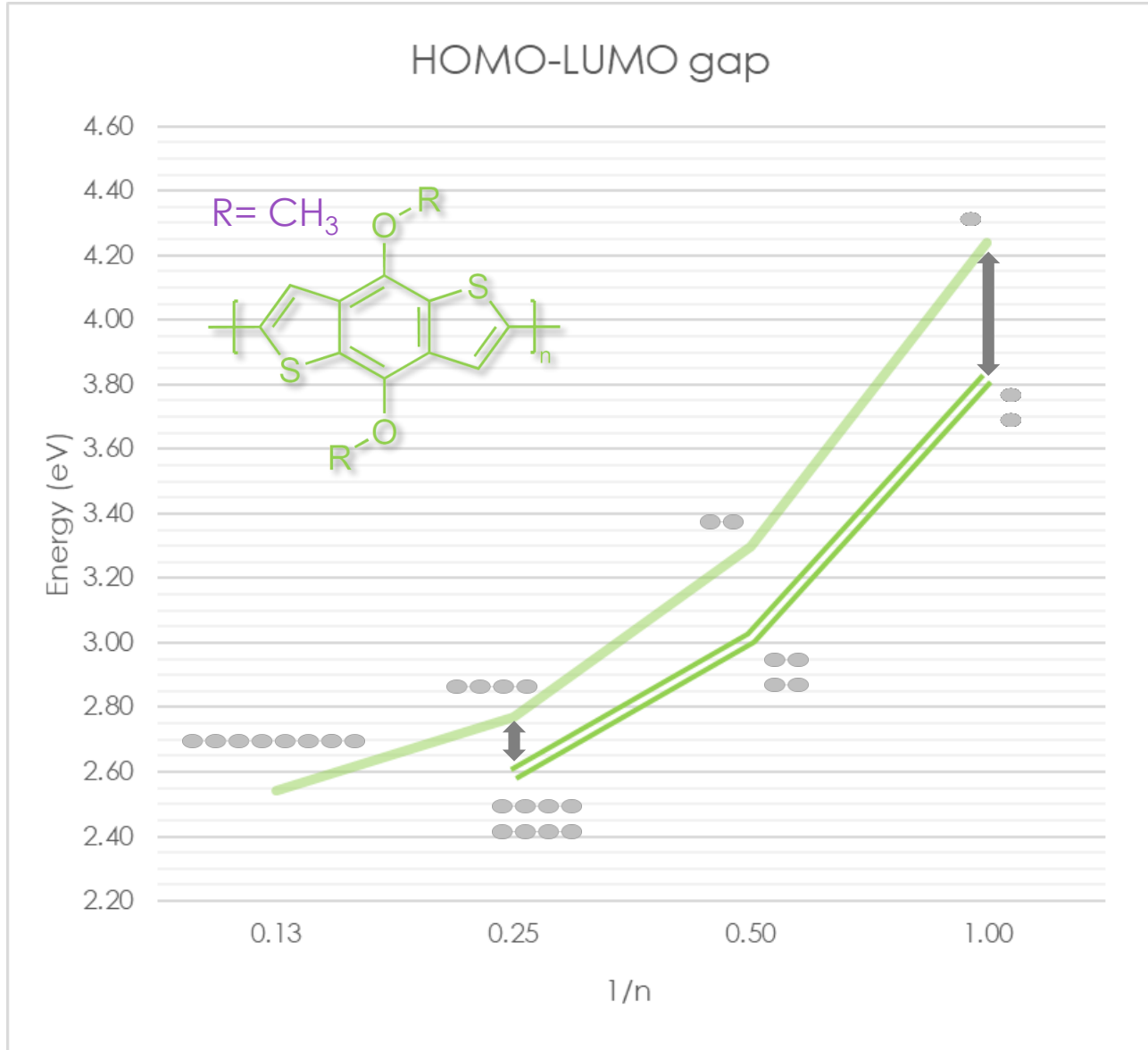
# Nature of blocks

# Side chains

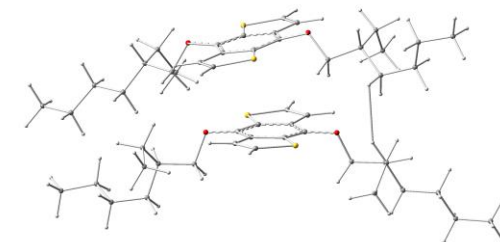
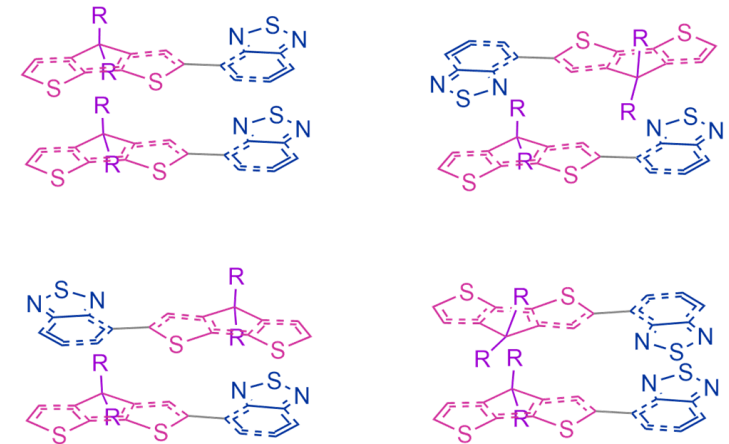
# Double chains







Conformations for 1u:



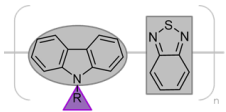
# Conclusion



Conjugation length: same trend of  $E_g^{HL}$  and  $E_g^{OPT}$



Nature of blocks: mixing blocks tunes properties



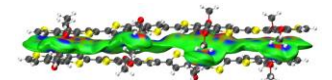
Side chains: negligible effect in isolated chain



It is important to consider other interactions!

## Perspectives

Noncovalent interactions analysis using Multiwfn/VMD

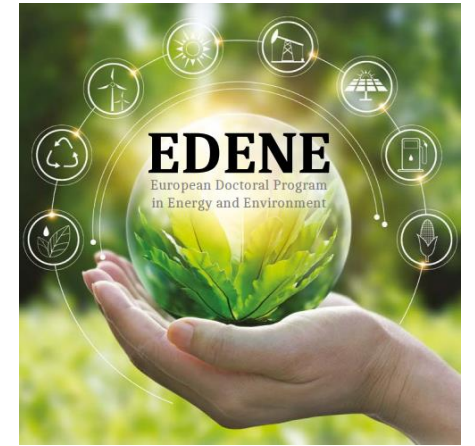


Trends of exciton binding energy





HPC resources from:



Pyrene cluster



Jean-Zay supercomputer  
IDRIS

Institute for Development and Resources  
in Intensive Scientific Computing



Mésocentre de Calcul Intensif Aquitain

Curta cluster

✉ [gm.aibara-paschoal@univ-pau.fr](mailto:gm.aibara-paschoal@univ-pau.fr)