Bio-sourced semiconducting organic materials : BIORG-EL

Roberto Lazzaroni

Laboratory for Chemistry of Novel Materials

University of Mons

GREENWIN conference
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LE FONDS EUROPÉEN DE DÉVELOPPEMENT RÉGIONAL, LA WALLONIE
ET LA FÉDÉRATION WALLONIE-BRUXELLES INVESTISSENT DANS VOTRE AVENIR

Low Carbon Footprint Materials

A research network on the
valorization of natural resources for
the fabrication of novel bio-sourced materials

5 universities

LIÈGE université · ULB · UMONS Université de Mons · UCLouvain · UNIVERSITÉ DE NAMUR

6 research centers

MateriaNova MATERIALS R&D CENTRE · Cenaero · celabor · certech centre de ressources technologiques en chimie · CENTEXBEL · sirris

with the support of

GREEN WIN CHEMICAL ENGINEERING & MATERIALS IN WALLONIA

Low Carbon Footprint Materials

Structure of the network: 3 research lines

1. BIOMAT

Building blocks from biomass for new polymer materials

2. MACOBIO

Bio-sourced composite materials

3. BIORG-EL

Bio-sourced semiconducting organic materials

BIOMAT activities : an example

Coordinator: Rosica Mincheva (Rosica.MINCHEVA@umons.ac.be)

Biomass

Miscanthus

Poplar

Willow

Local
Abundant

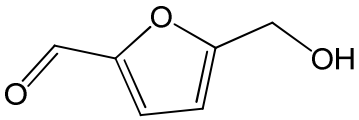
Treatment

- NaOH / eutectic mixture
- Organosolv / eutectic mixture

Simpler protocol

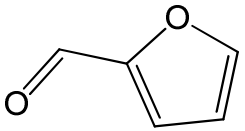
- Water consumption < 15%
- Working temp. < 90°C

Building blocks



5-HMF
(80%)

PET+PEF



2-F
(+/- 80%)

Lignin and other building blocks (> 50%)

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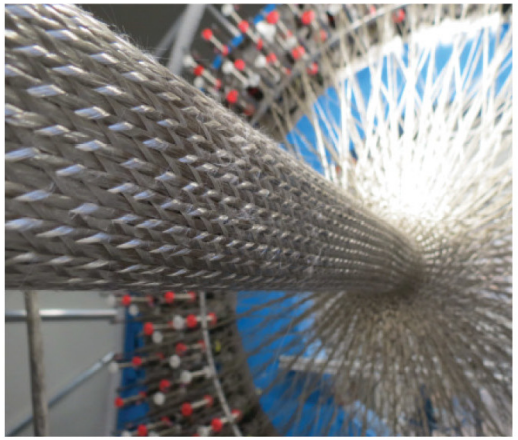
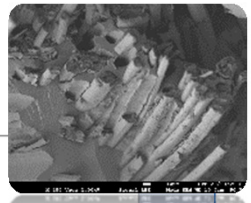


3. BIORG-EL
Bio-sourced semiconducting organic materials

MACOBIO : the concept

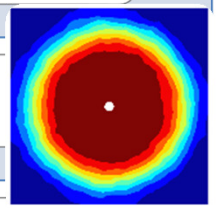
Coordinator: David Dumas (david.dumas@cenaero.be)

- Modification of polymer materials with bio-sourced charges



- Processing and surface treatment of short and long fibers

- Sustainable processing approach (↘ energy ↘ solvents ↘ toxicity)
- Materials modeling for a robust design



- Performance characterization of bio-sourced composites

- Ecodesign, including LCA
- Short production and delivery circuits for technical products

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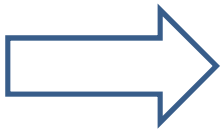
Why organic semiconductors ?

Combination of

- Optical and electronic properties of semiconductors
- Chemical and mechanical properties of polymers
  (flexibility, lightweight, tunability)



'Organic Electronics'

Application domains

1. Display and lighting technologies: 'OLED'

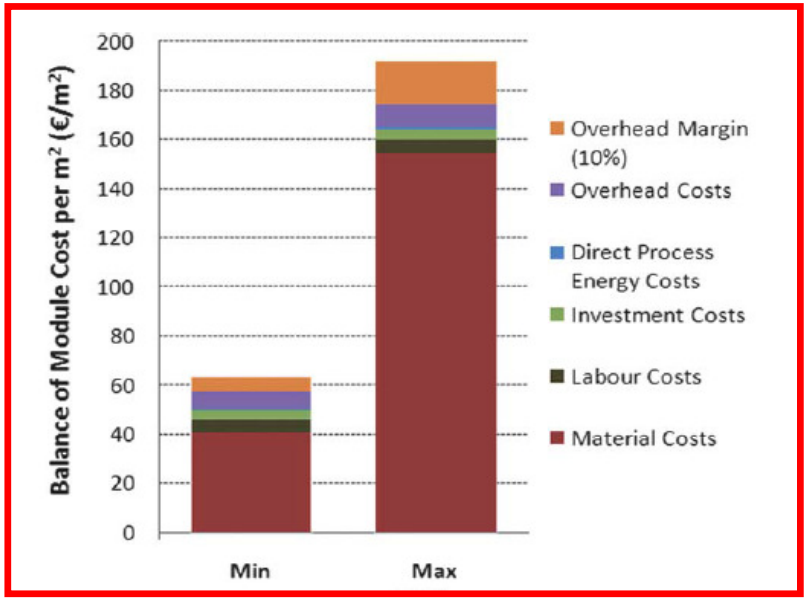
2. Photovoltaic technologies : OPV, DSSC, hybrids

3. Photocatalysis: 'water splitting', 'solar fuels'

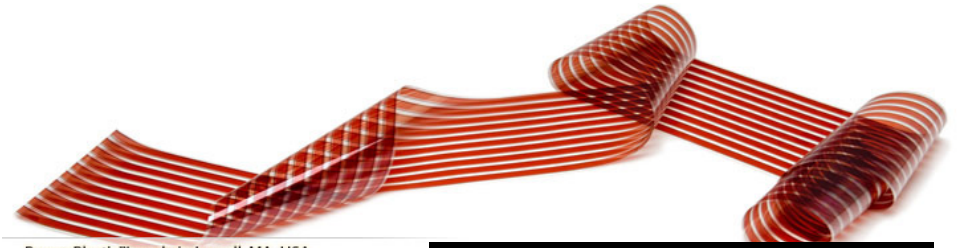
Organic semiconductors for energy applications

Displays

Lighting



Solar cells



Konarka Power Plastic

The cost of the materials has a major impact

BIORG-EL: the goal

Developing new bio-sourced or bio-inspired materials for organic electronics

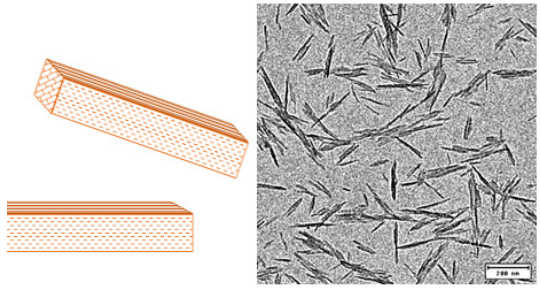
Two functions :

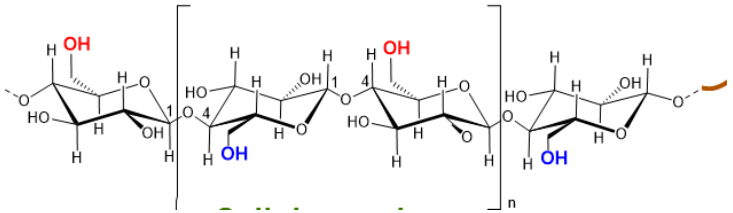
1. Light absorption/emission

2. Functional substrates for active layers

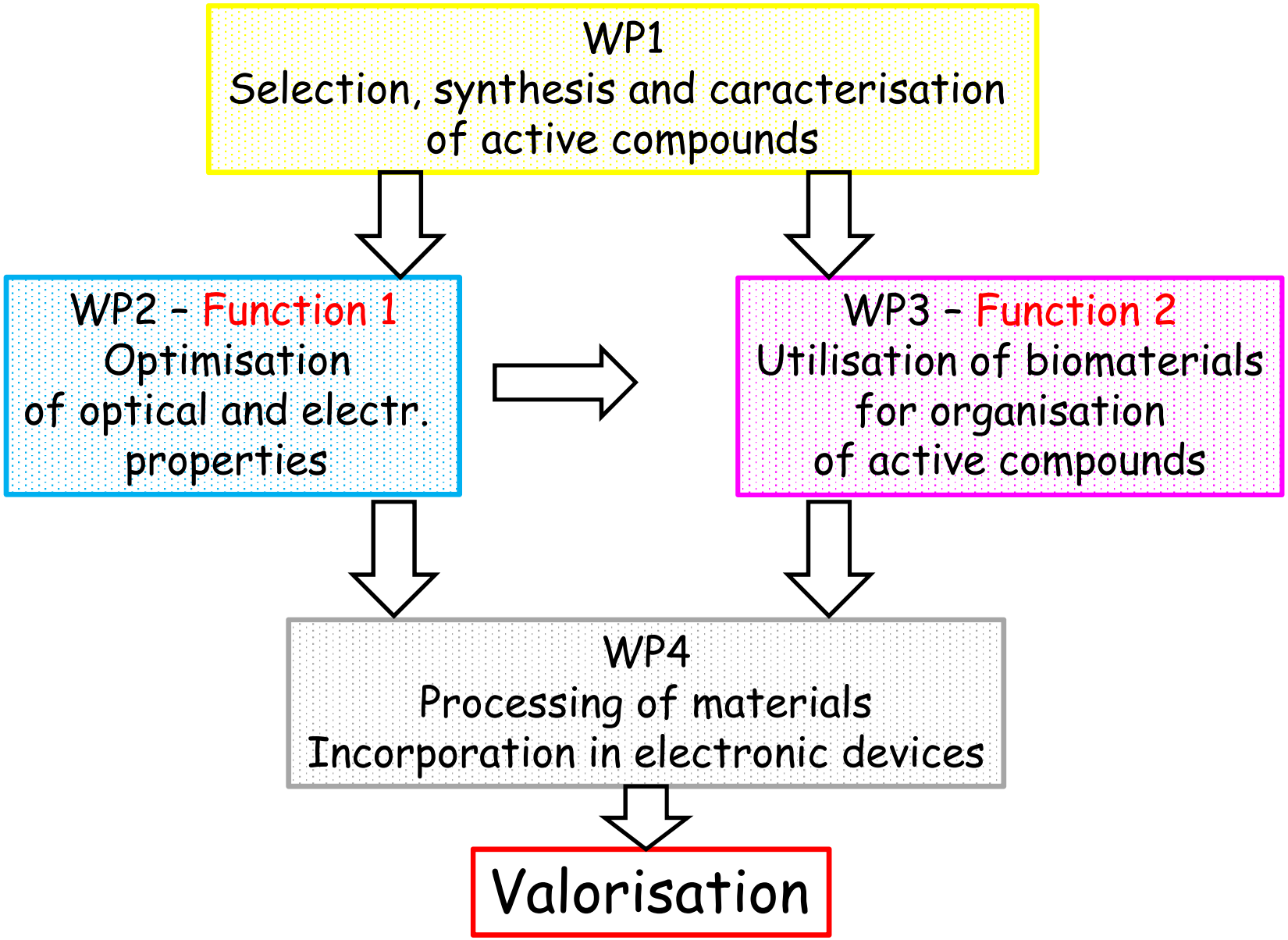
Dyes extracted from biomass

Cellulose nanocrystals





BIORG-EL : the research strategy



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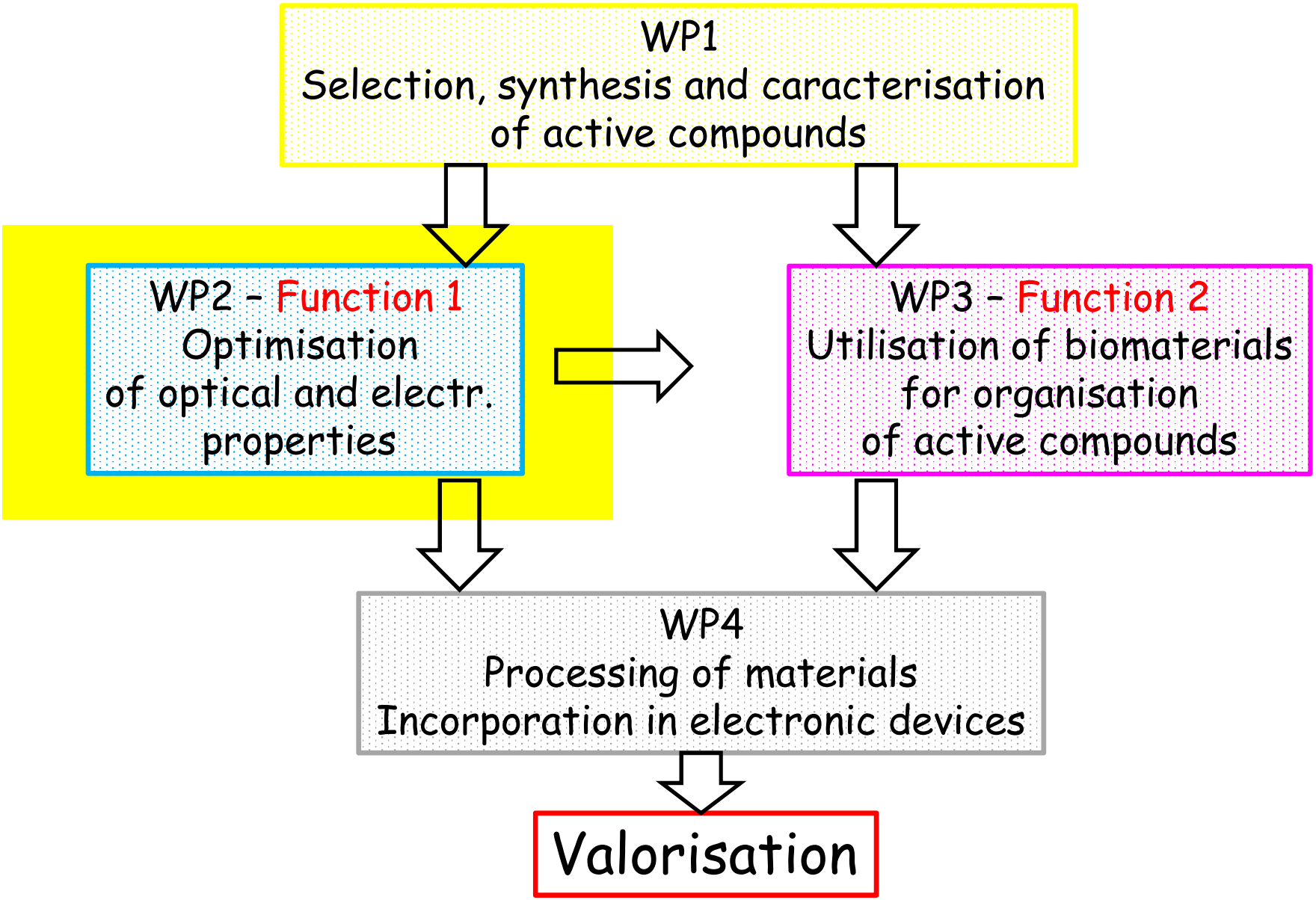


Bio-sourced compounds for dye-sensitized solar cells

1. Assessing the potential of dyes with quantum-chemical modeling

	HOMO (eV)	LUMO (eV)
Bilirubin	-4.95	-2.13
	-5.01	-2.19
Phycocyanin	-4.62	-2.23
	-4.88	-2.59
Phycocyanobilin	-4.59	-2.33
	-4.83	-2.65
Biliverdin	-4.87	-2.82
	-5.07	-3.03

B3LYP / 6-31G**
Solvent = water

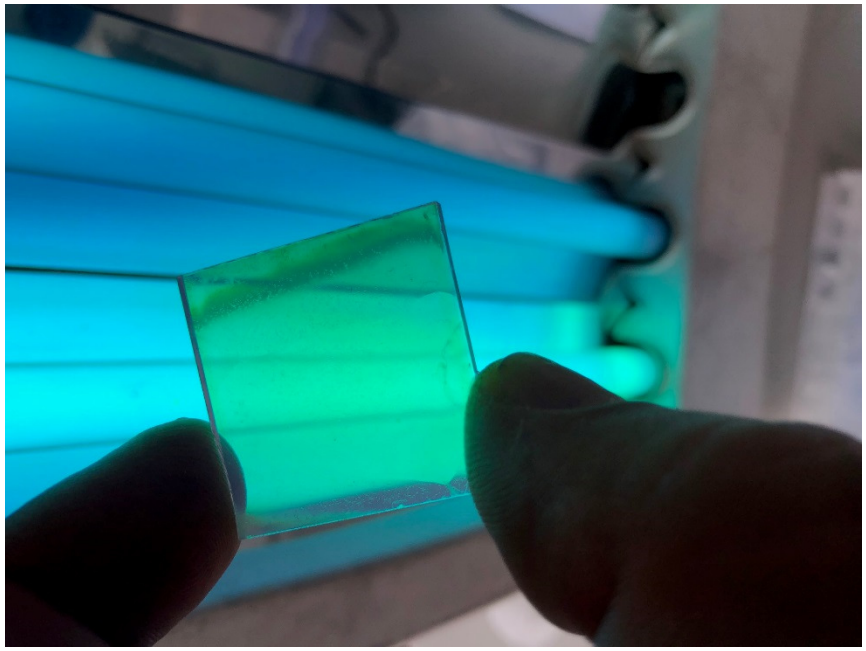
LUMO level of all the dyes above the CBE of TiO_2

Promising as active layer in DSSC

Phycocyanine appears as an interesting candidate

2. Extracting the dyes from spirulina - Materia Nova Biotech

3. Phycocyanine dye impregnated in TiO_2 electrode on glass



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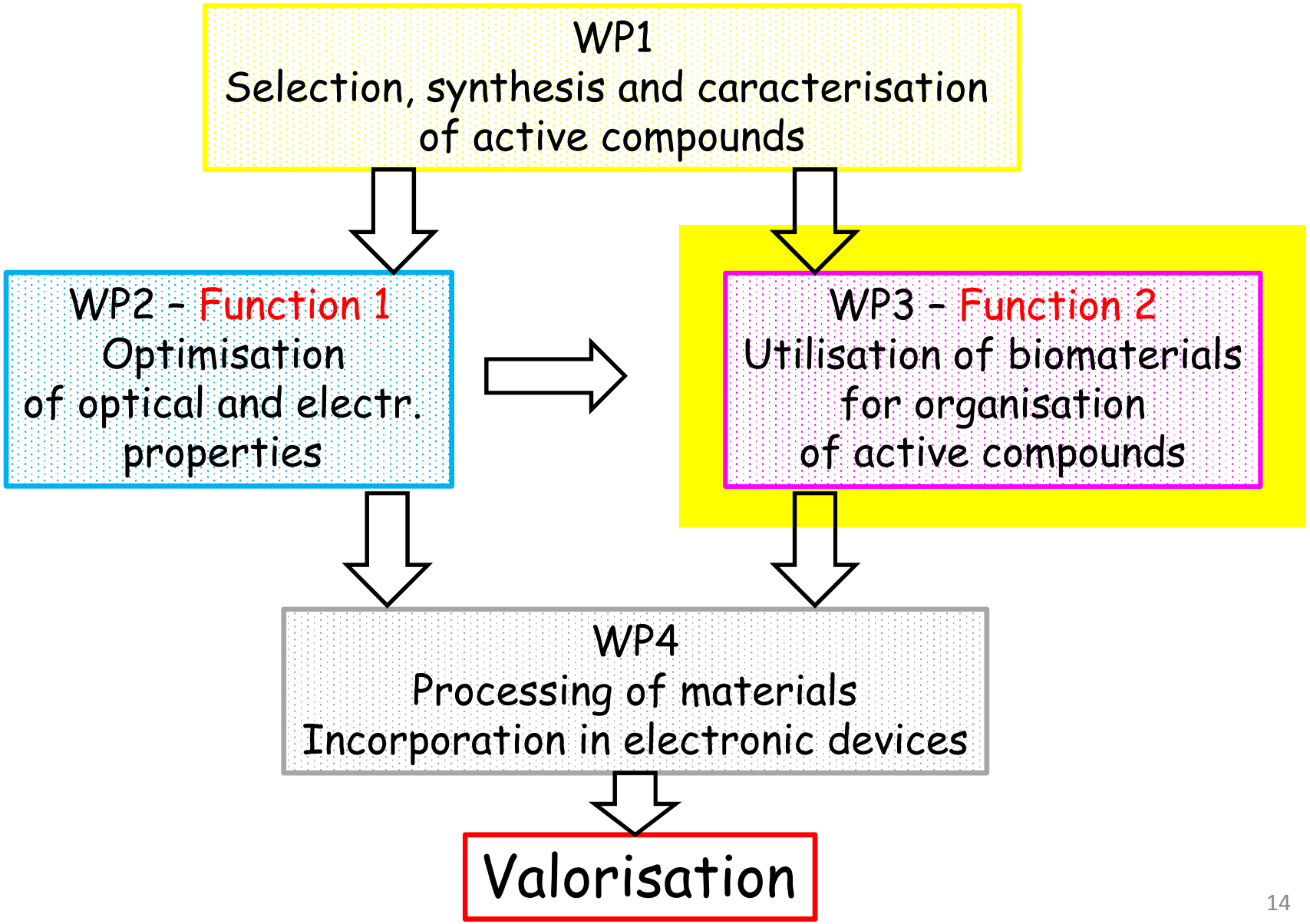
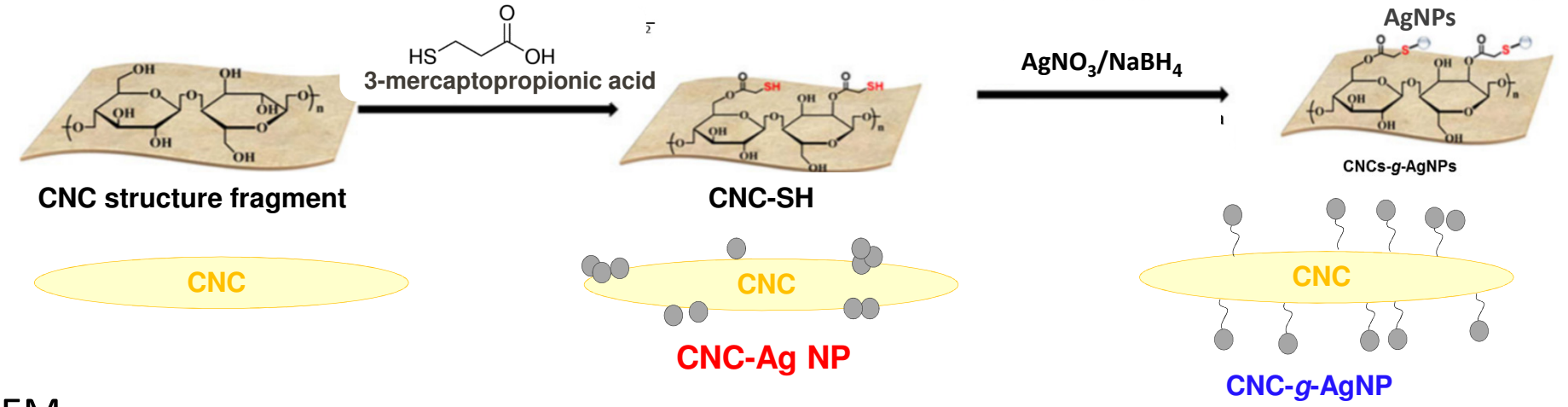
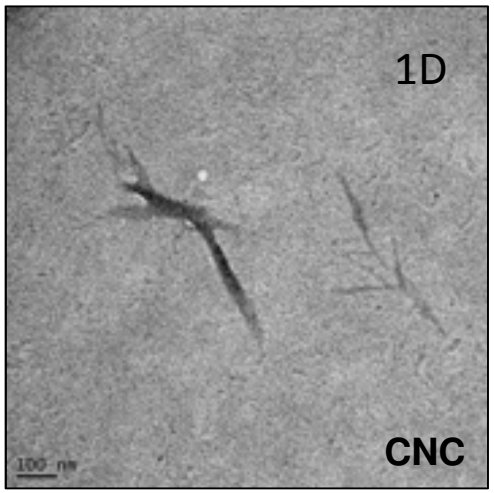


Nanocellulose as functional substrate

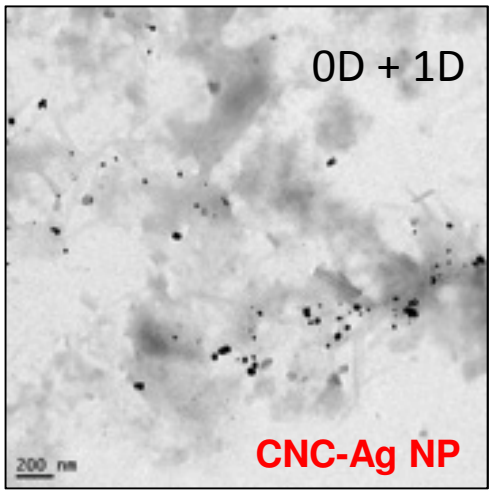
Ag nanoparticles as scattering centers for light in devices



TEM

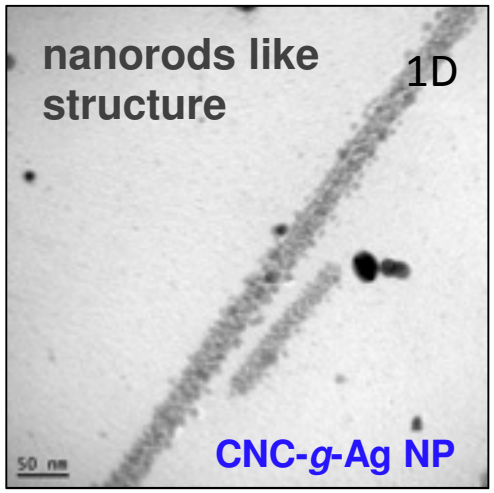


Nanocrystals length 150 nm



Adsorbed AgNPs 8 nm

randomly dispersed

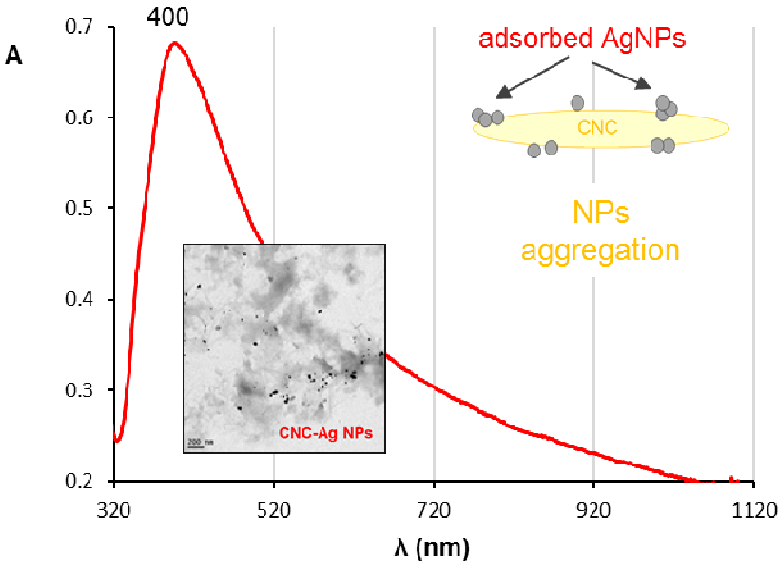


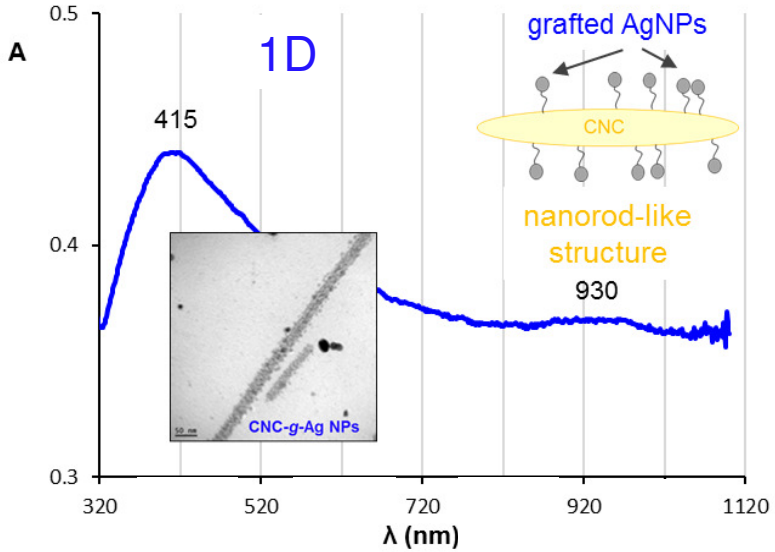
Grafted AgNPs 14 nm

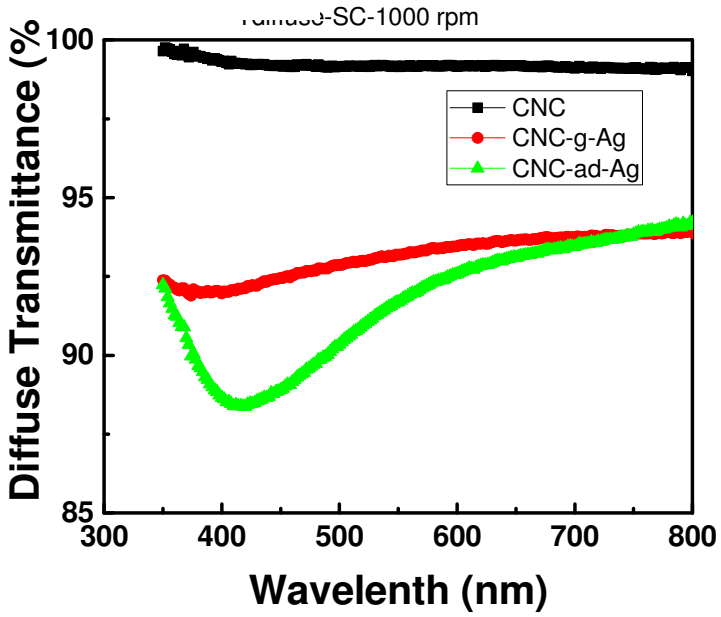
regularly organised

Nanocellulose as functional substrate

Optical properties of Ag NP – CNC hybrids







Ag nanoparticles on CNC absorb and scatter visible light

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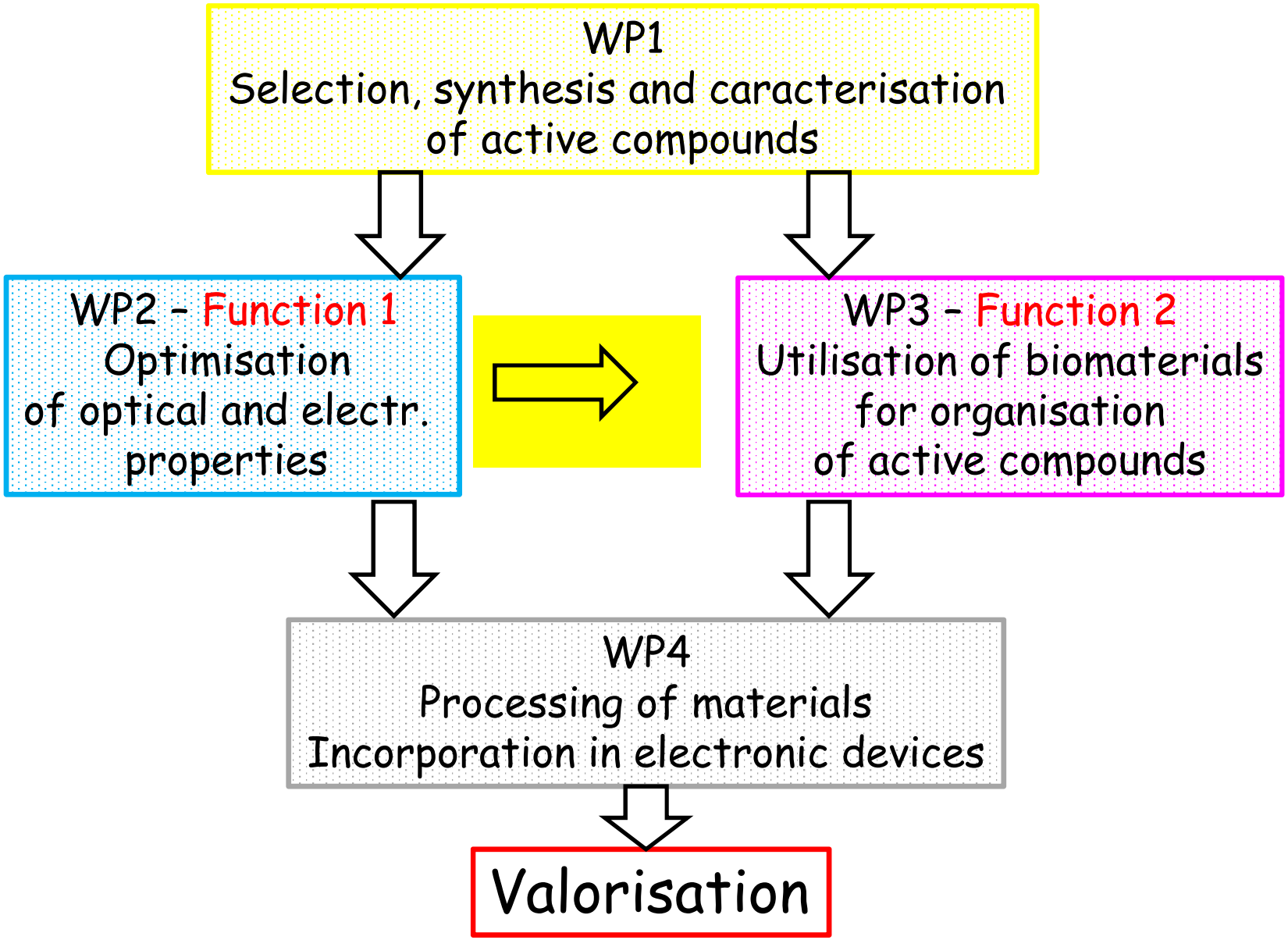
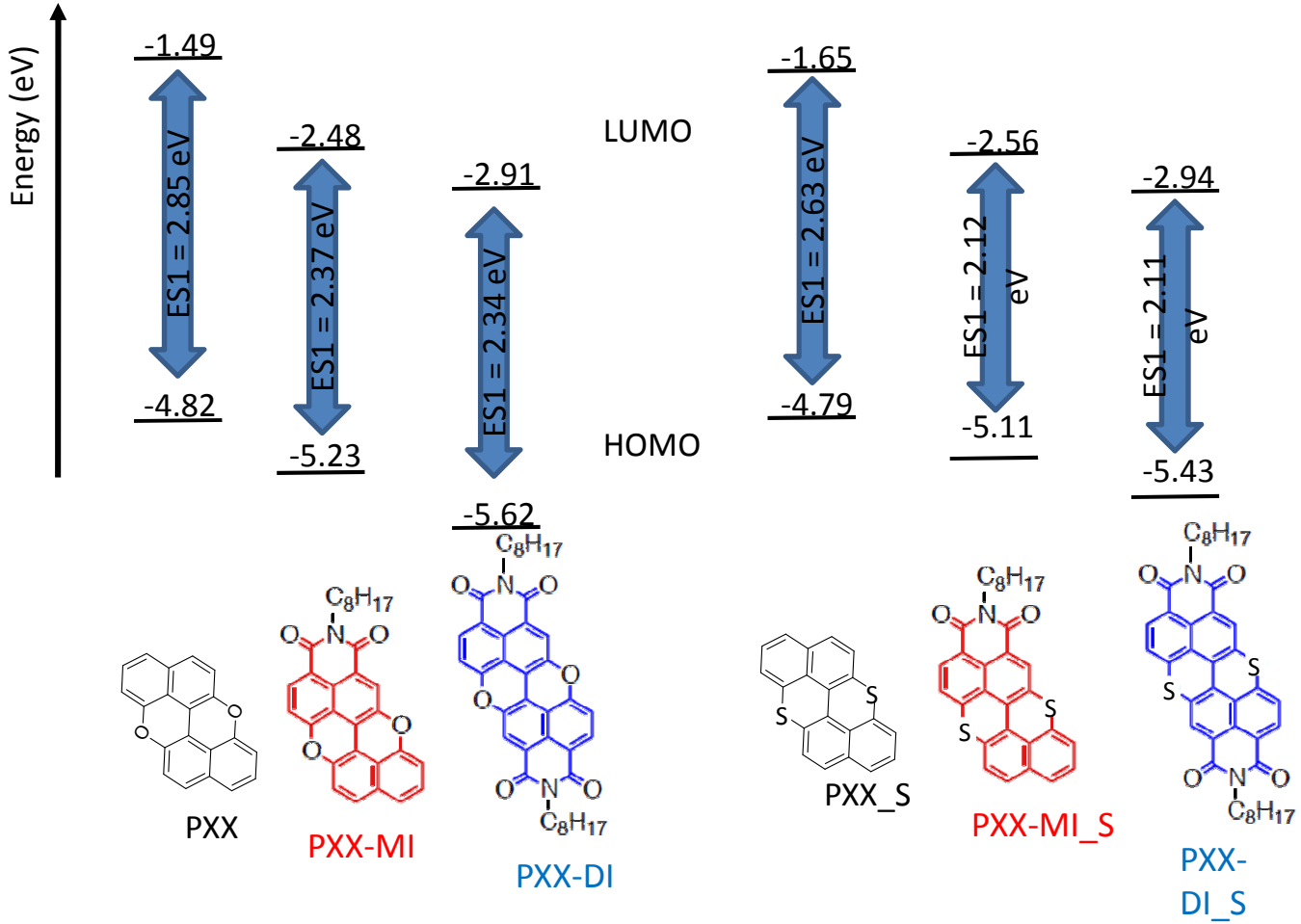
Incorporation in photovoltaic cells ?

BIORG-EL : the research strategy



Development of bio-inspired chromophores

Modeling the electronic properties of PXX dyes



Smaller HOMO-LUMO energy gap for the sulfur derivatives

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Sulfur derivatives absorb at lower energy

One imide group is sufficient

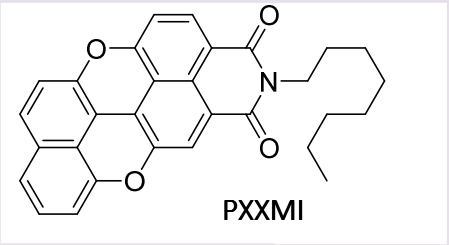
Oxygen dyes

Sulfur dyes

TD-DFT (B3LYP / 6-31G** / dichloromethane)

Development of bio-inspired chromophores

Synthesis and optical properties



PXXMI

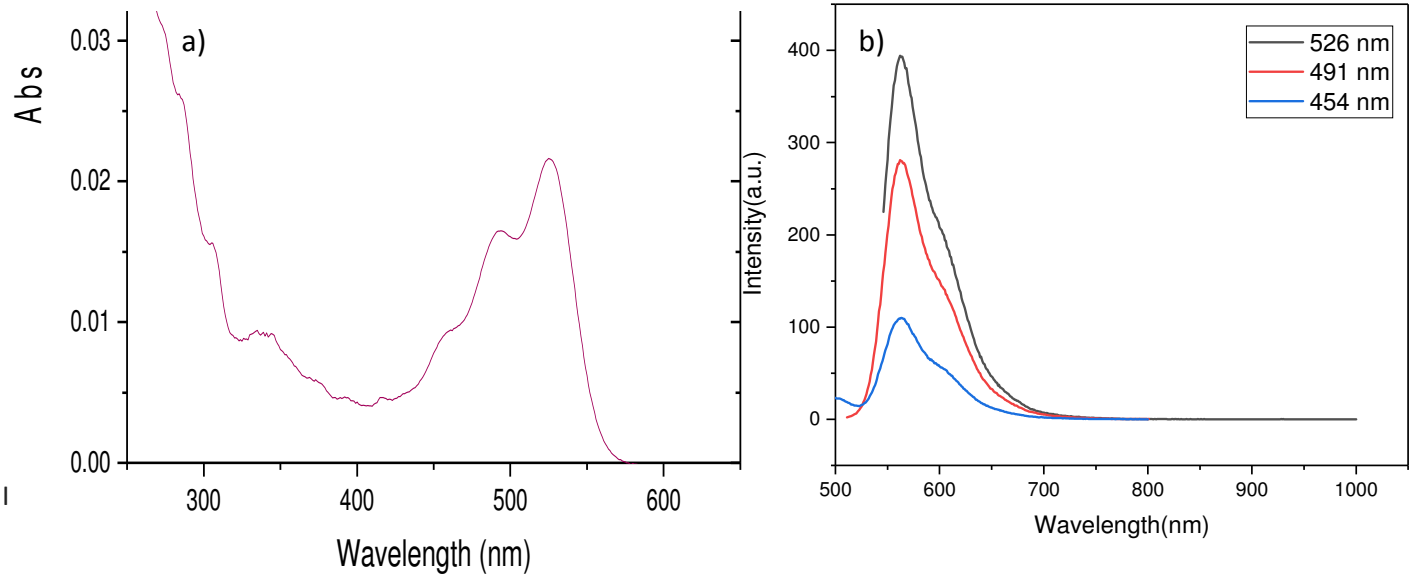
- Synthesis of the octyl-PXXMI chromophore
- Target compound in homogeneous phase to evaluate the **photocatalytic activity**
- Activity compared with heterogeneous catalysts


Red powder

Strong absorption in visible

Light emission in visible

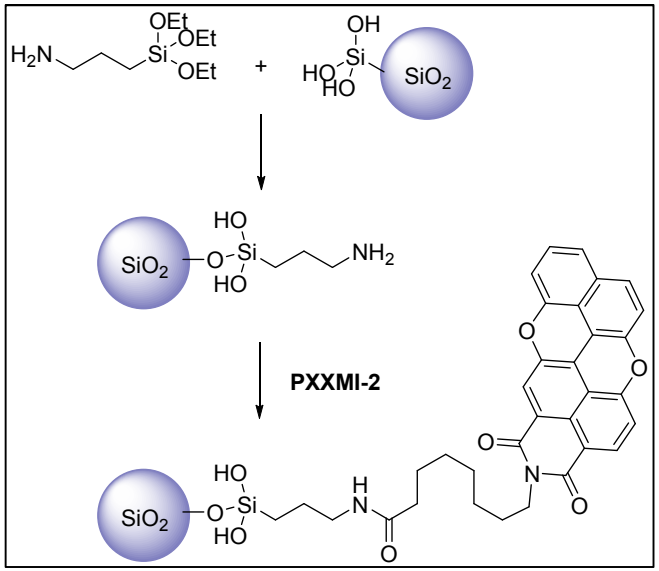

Photo of the solution of PXXMI ($3.0*10^{-6}$ M in CH_2Cl_2)

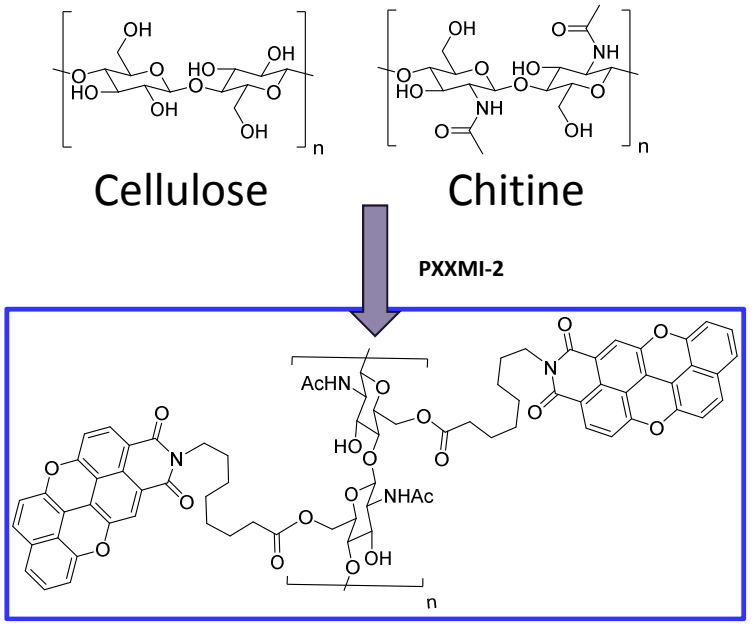


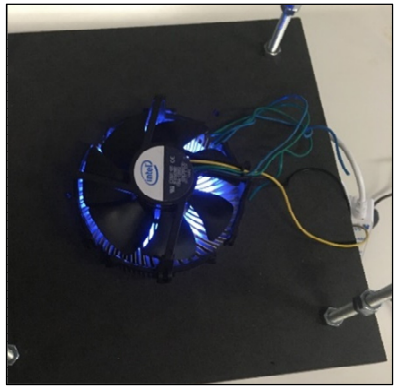
Absorption (a) and emission (b) spectra of PXXMI ($3.0 \cdot 10^{-6}$ M in CH_2Cl_2)

Chromophores on functional substrates

Functionalization of bio-sourced supports with the PXXMI derivatives







BIORG-EL partnership

Service de Chimie des Matériaux Nouveaux
R. Lazzaroni et al., coordinator

Service des Matériaux Polymères et Composites
J.M. Raquez, R. Mincheva, Ph. Dubois et al.

Laboratoire de Chimie des Matériaux Appliqués
C. Aprile et al.

+ collab. with D. Bonifazi et al. (UCardiff)

Unité de Chimie des Matériaux Nouveaux
P. Viville et al.