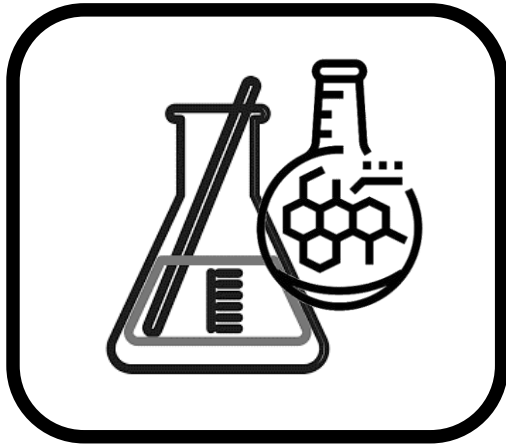


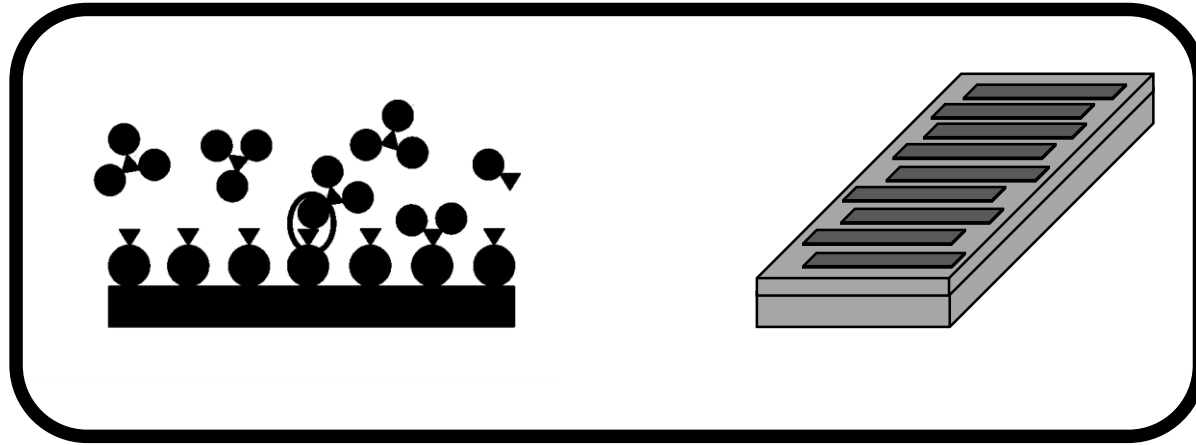
## Outlook for curcuminoids as sensors and electronic elements



# Guidelines

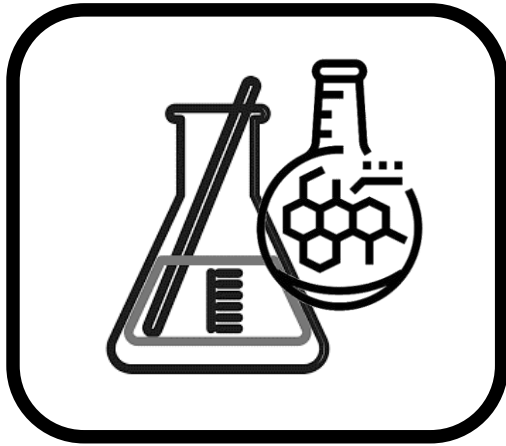


Synthesis

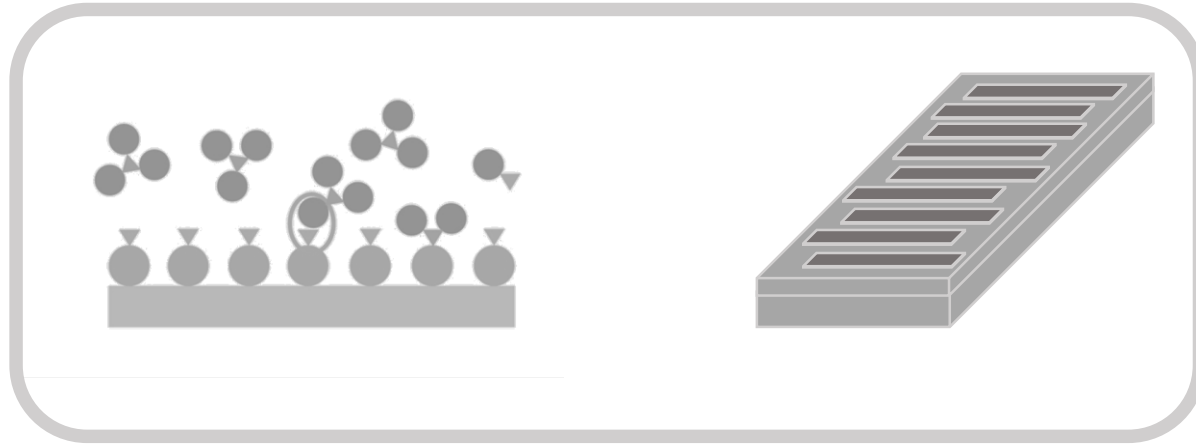


Deposition methods & Measurements

# Guidelines



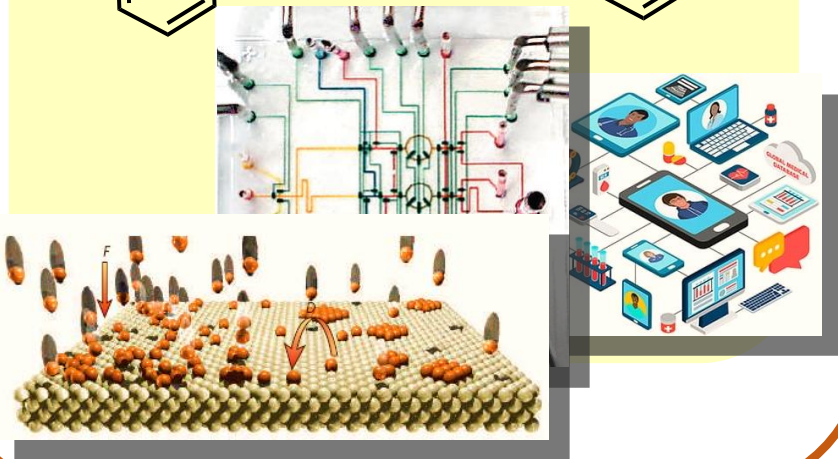
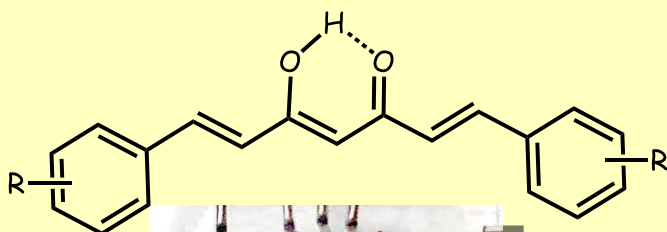
Synthesis





# Curcuminoids (CCMoids)

## Nanoscience/Nanotechnology



## Symmetric CCMoids

Diarylheptanoid skeleton  
Keto-enol moiety  
Aromatic rings  
Additional groups

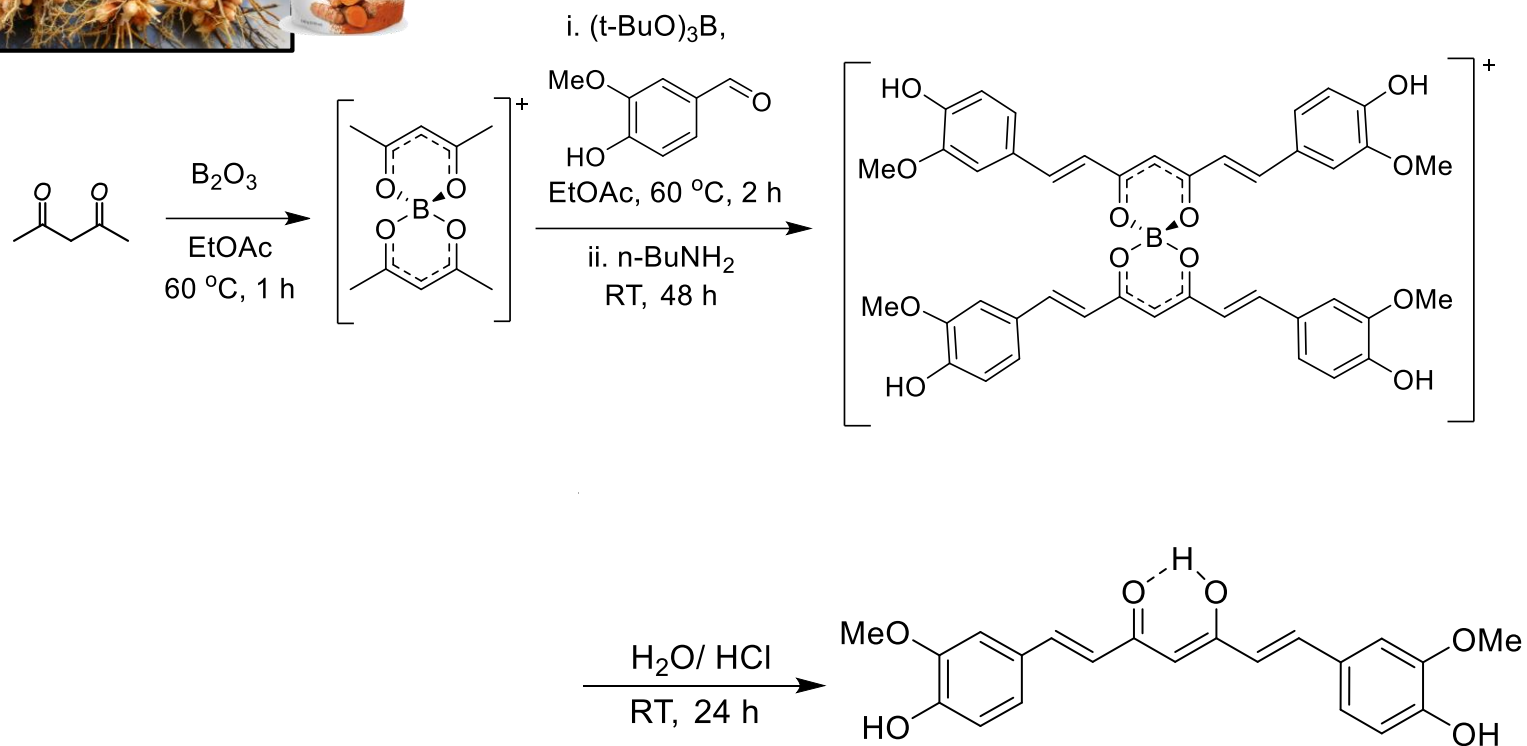
## Synthetic procedure: Pabon's method

Single pot reaction  
Straightforward purification  
High yields

## CCMoids Properties

Linear conjugated systems  
Coordination units / heteroditopic linkers  
Dyes  
Fluorophore and solvatochromic molecules  
Antiinflammatory and antioxidant agents

# Synthesis of curcumin (CCM)



**Synthetic procedure:  
Pabon's method**

Single pot reaction  
Straightforward purification  
High yields





# Examples of CCMoids with FunNanoSurf

Organic solar cells

Coordination Polymers & MOFs

Single-molecule magnets

Gels

Molecular electronics

## Collaborators:

Prof. Luis Echegoyen

Prof. Eliseo Ruiz

Prof. Herre van der Zant

Prof. Maria Lluïsa Perez-Garcia

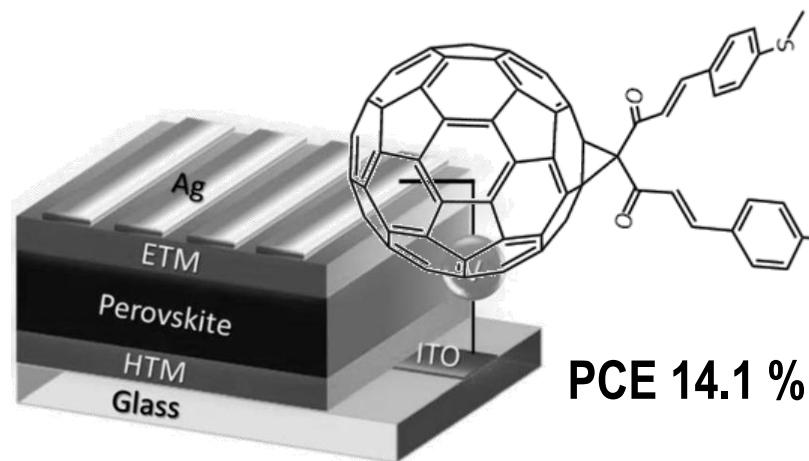
Dr. Mònica Soler-Jaumà

Dr. Diana Dulić

Dr. Concepción Domingo

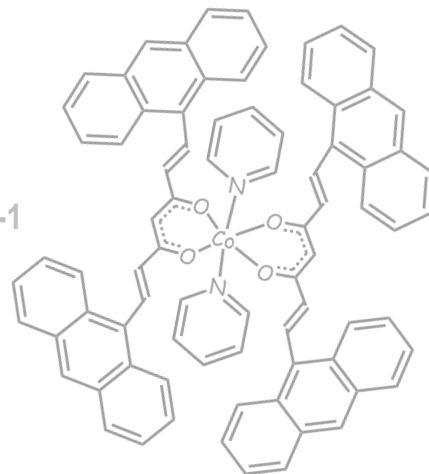
Dr. José P. Giner

## Perovskite Solar Cells

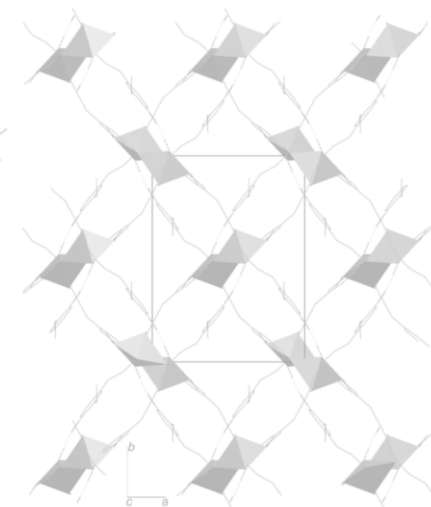
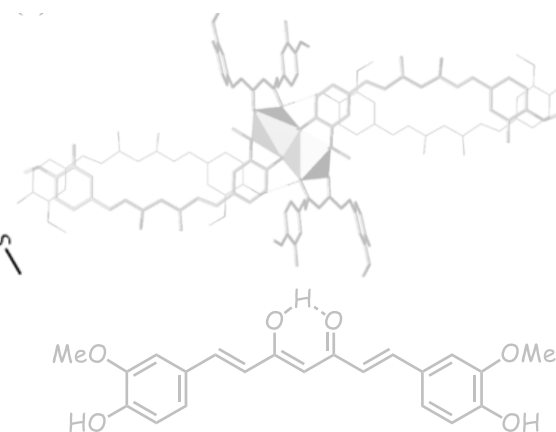


## SMMs

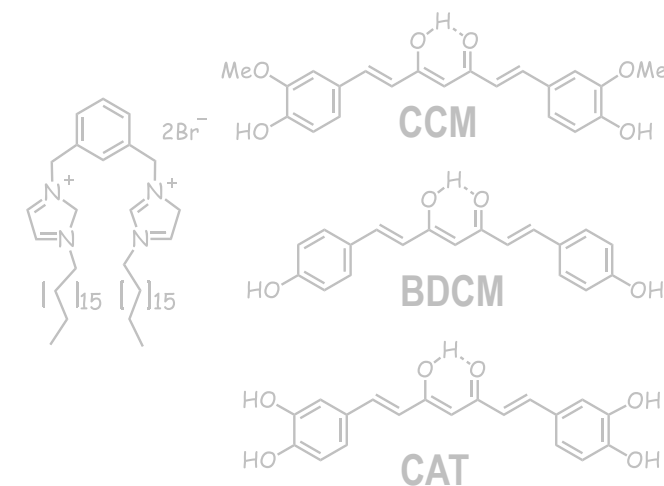
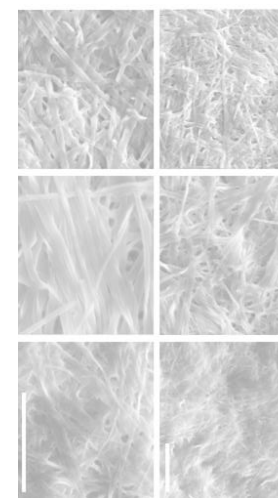
$D = -74 \text{ cm}^{-1}$



## bioMOFs



## Gels





# Examples of CCMoids with FunNanoSurf

Organic solar cells

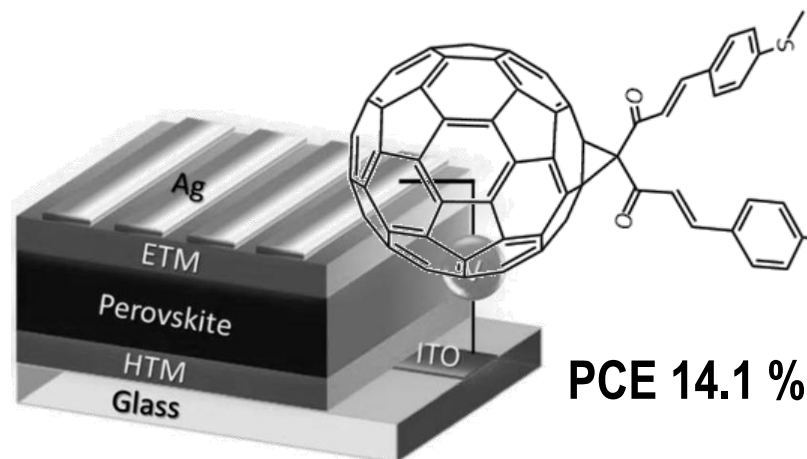
Coordination Polymers & MOFs

Single-molecule magnets

Gels

Molecular electronics

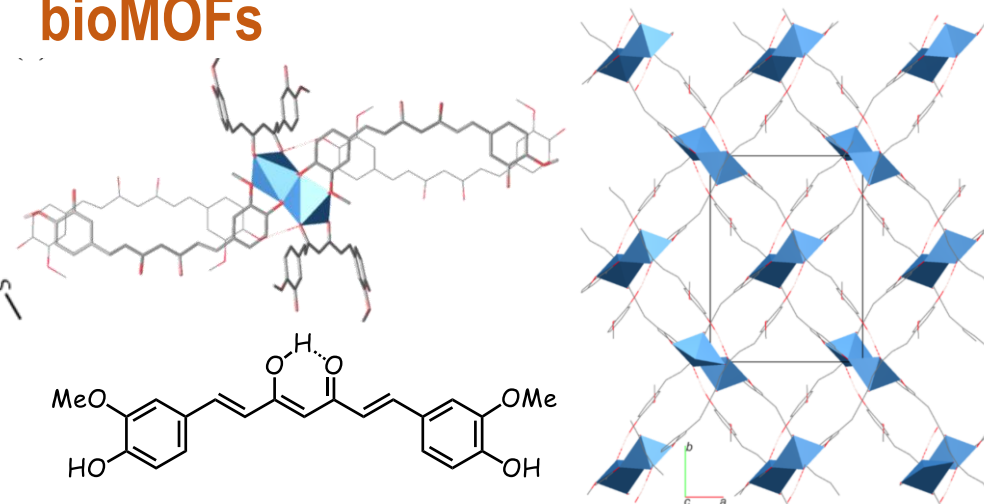
## Perovskite Solar Cells



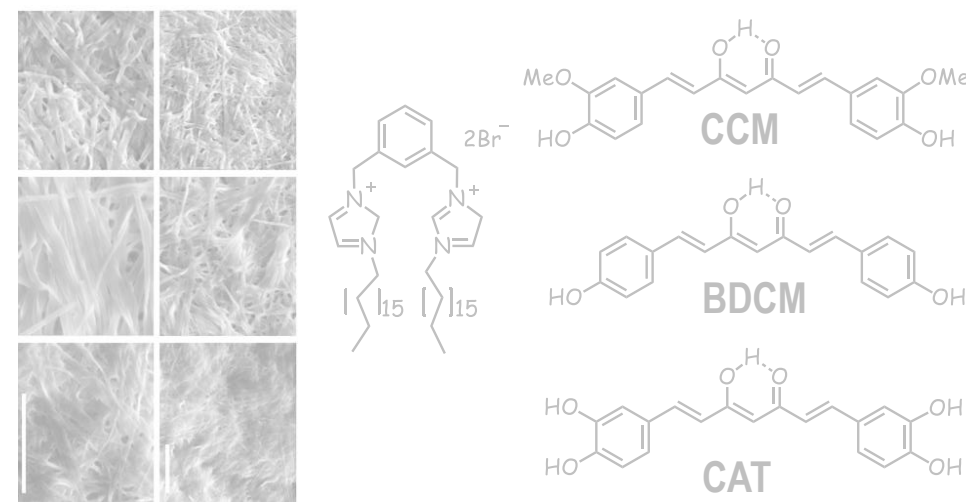
## SMMs



## bioMOFs



## Gels



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Dr. Mònica Soler-Jaumà

Dr. Diana Dulić

Dr. Concepción Domingo

Dr. José P. Giner

E. Castro *et al.* *RSC Advance* **2018**, 8, 41692; N. Portoles-Gil *et al.* *ACS Sustainable Chemistry & Engineering*, **2018**, 6, 12309. L. Rodríguez-Cid *et al.* **2020**, *Crystal Growth & Design*, 20, 6555; J. I. Olavarria-Contreras *et al.* *Chemical Science*, **2018**, 9, 6988. D. Limón *et al.* *ACS Applied Nano Materials* **2022**, an-2022-01482m.R1



# Examples of CCMoids with FunNanoSurf

Organic solar cells

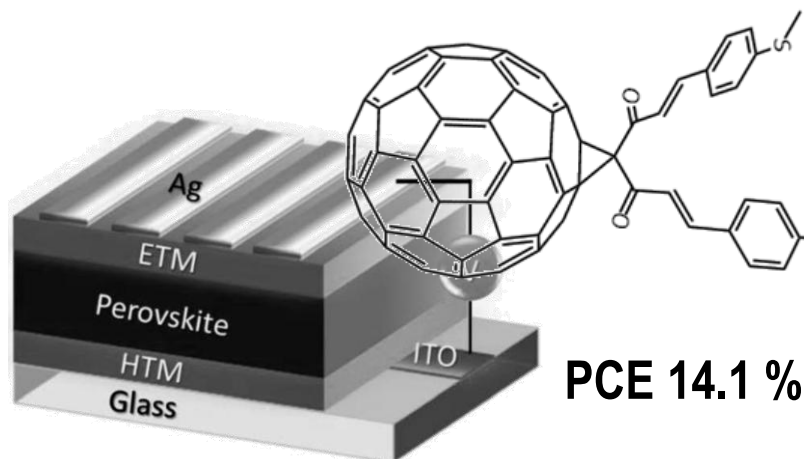
Coordination Polymers & MOFs

Single-molecule magnets

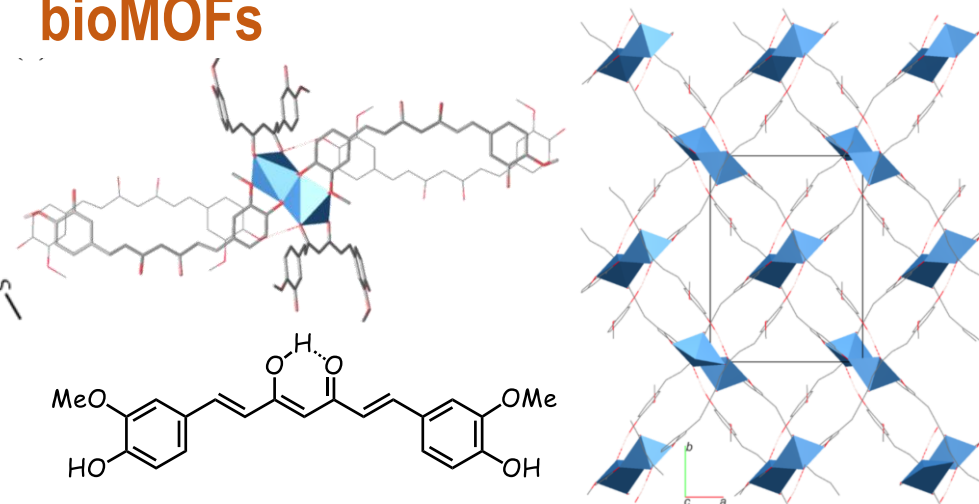
Gels

Molecular electronics

## Perovskite Solar Cells

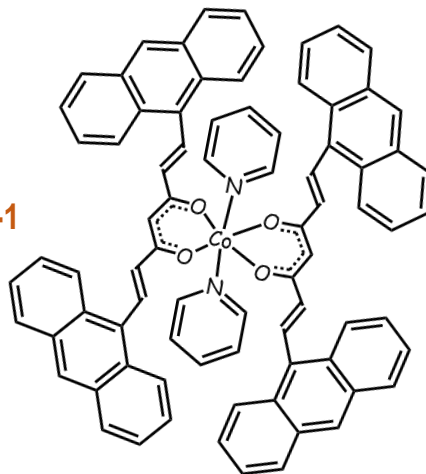


## bioMOFs

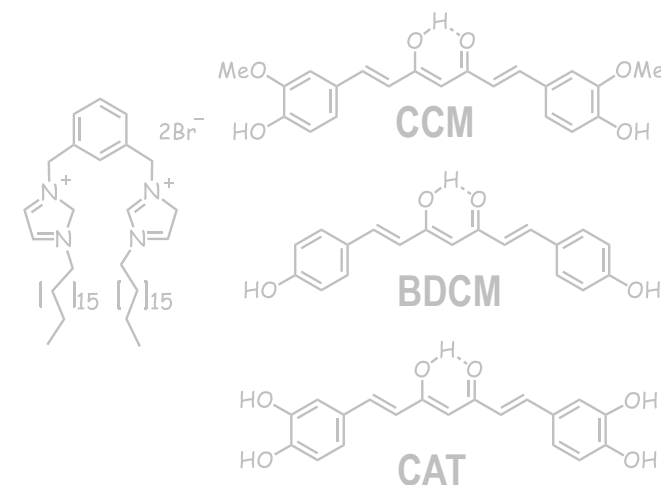
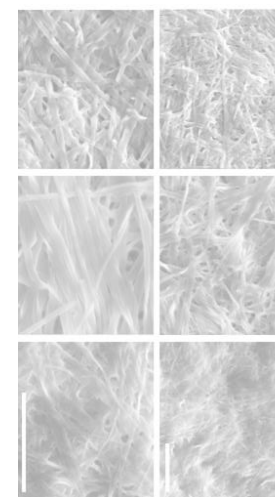


## SMMs

$D = -74 \text{ cm}^{-1}$



## Gels



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# Examples of CCMoids with FunNanoSurf

Organic solar cells

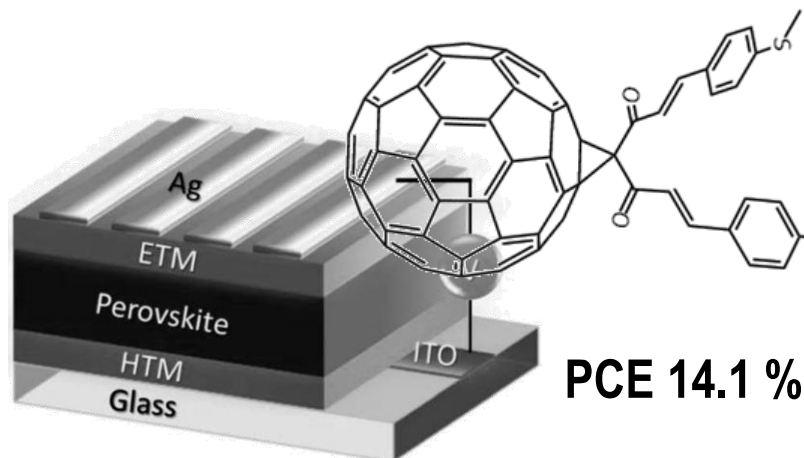
Coordination Polymers & MOFs

Single-molecule magnets

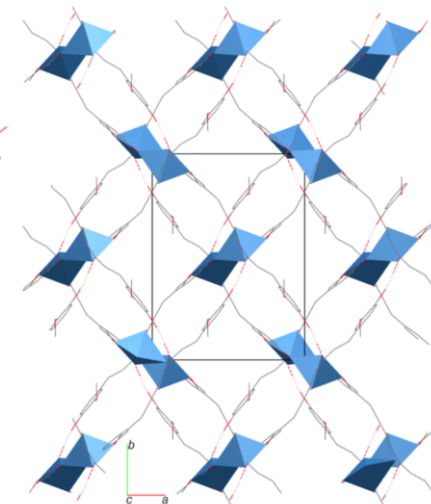
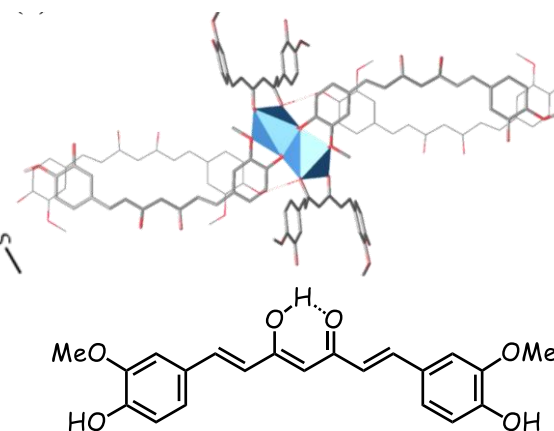
Gels

Molecular electronics

## Perovskite Solar Cells

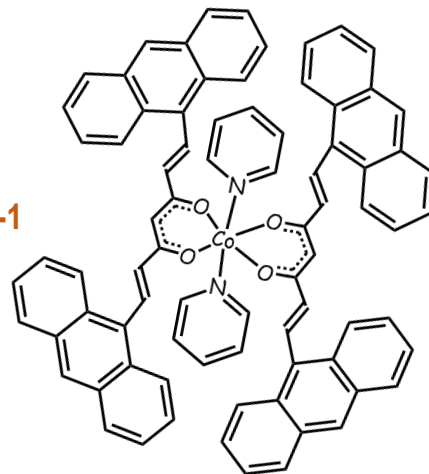


## bioMOFs

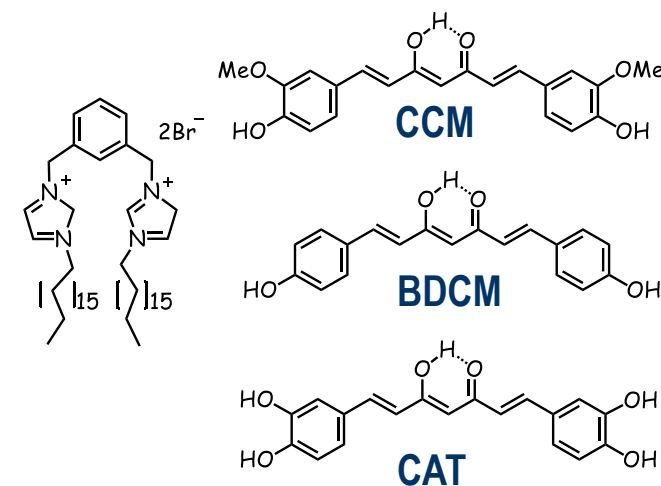
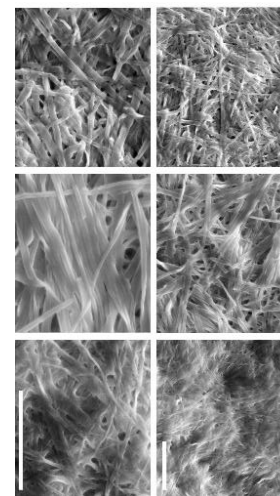


## SMMs

$D = -74 \text{ cm}^{-1}$



## Gels



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Dr. Diana Dulić

Dr. Concepción Domingo

Dr. José P. Giner



# Examples of CCMoids with FunNanoSurf

## Molecular Electronics - MCBJ

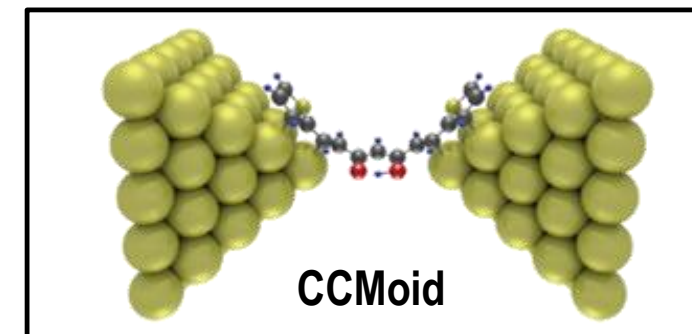
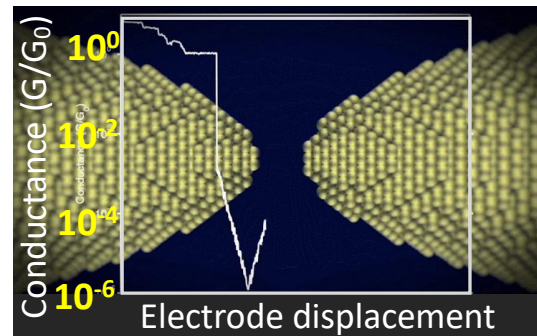
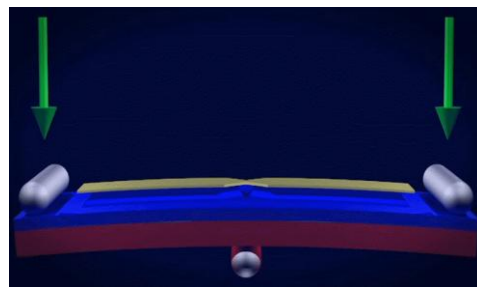
Organic solar cells

Coordination Polymers & MOFs

Single-molecule magnets

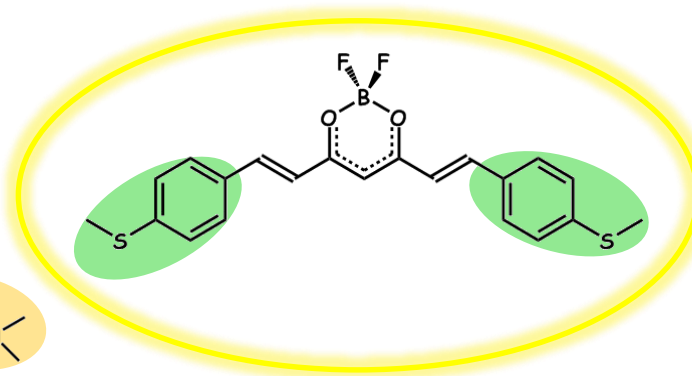
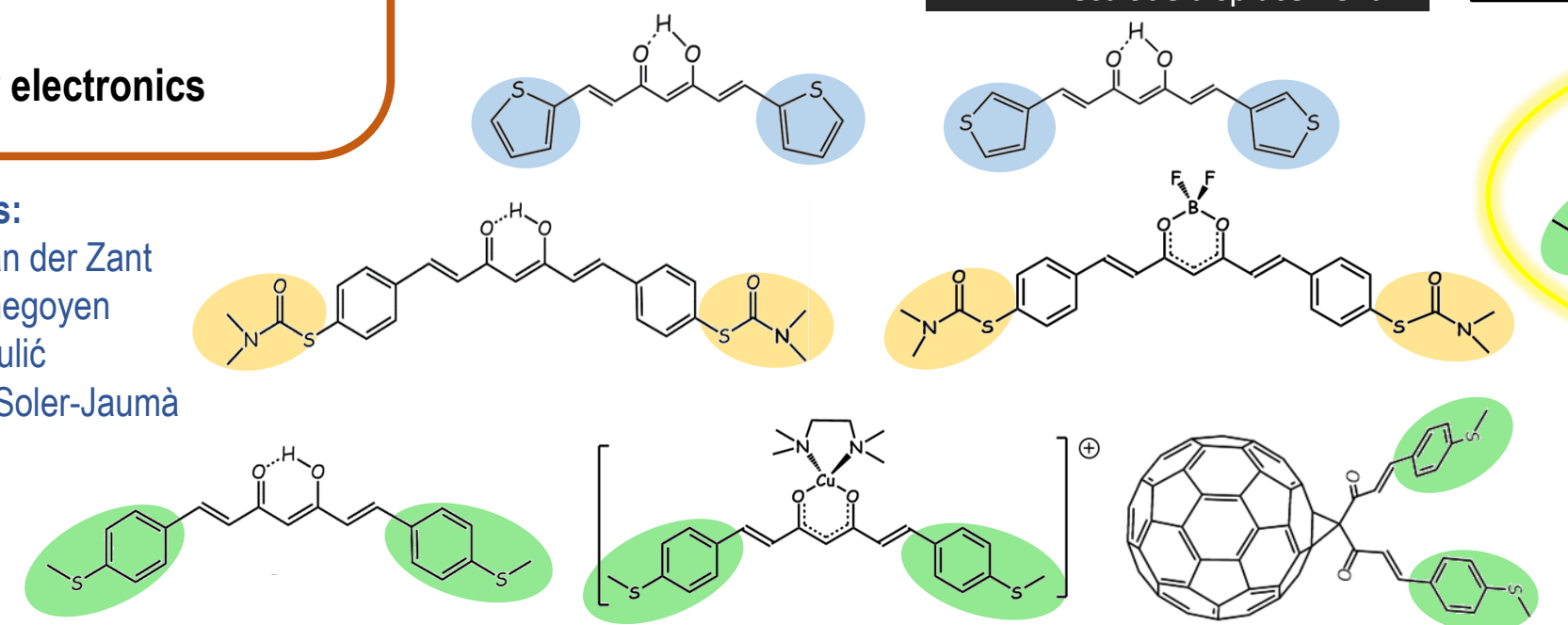
Gels

Molecular electronics



### Collaborators:

- Prof. Herre van der Zant
- Prof. Luis Echegoyen
- Dr. Diana Dulić
- Dr. Mònica Soler-Jaumà

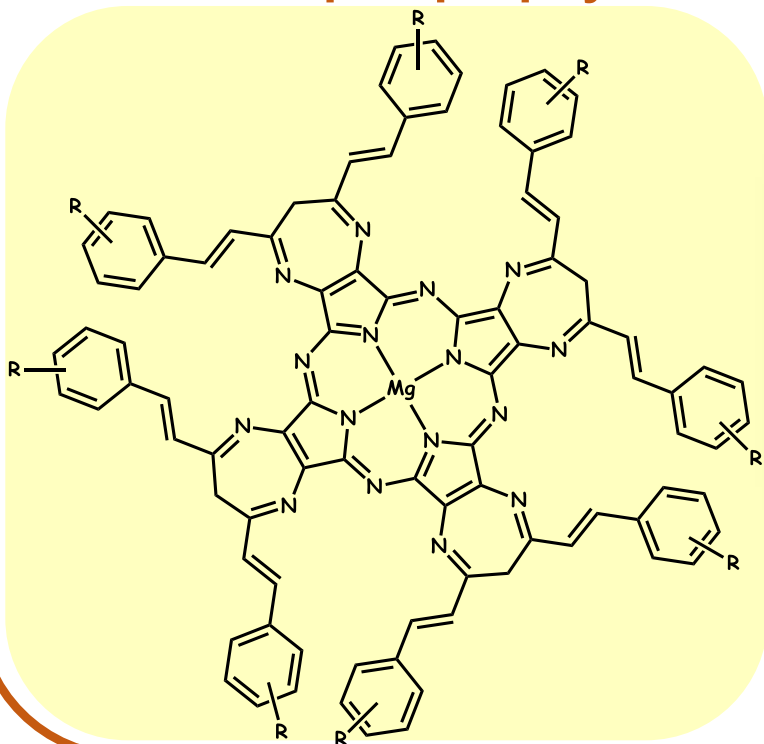


**Conductance values**  
 $5.4 \times 10^{-5} G_0$   
 $1.4 \times 10^{-4} G_0$

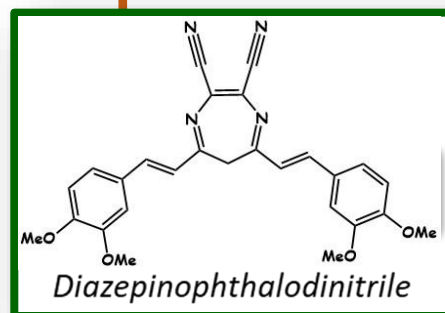
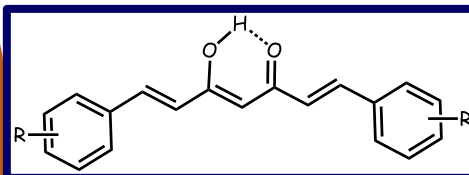


# CCMoids as starting materials

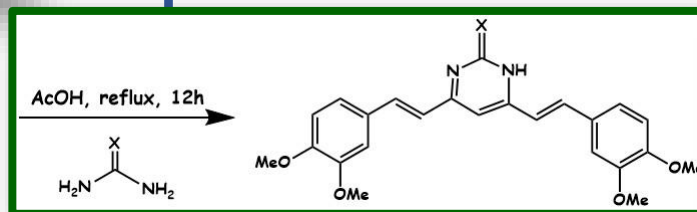
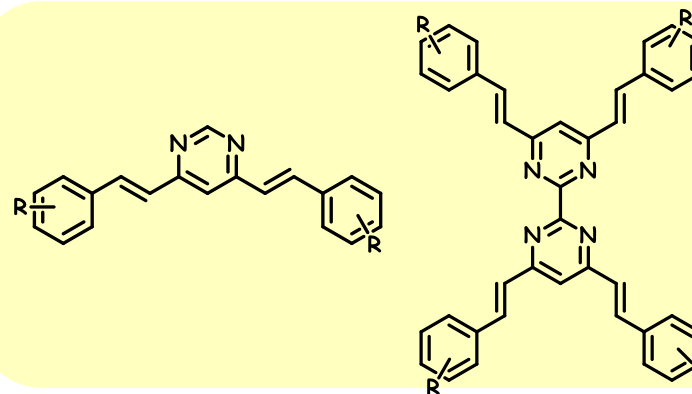
## Teradiazepinoporphyrazines



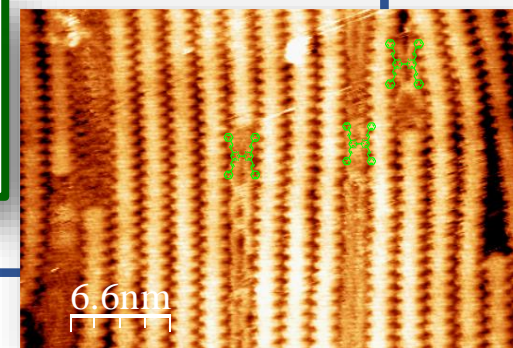
**FunNanoSurf:**  
Joseline Iribarra-Araya



## pyrimidines/bipyrimidines

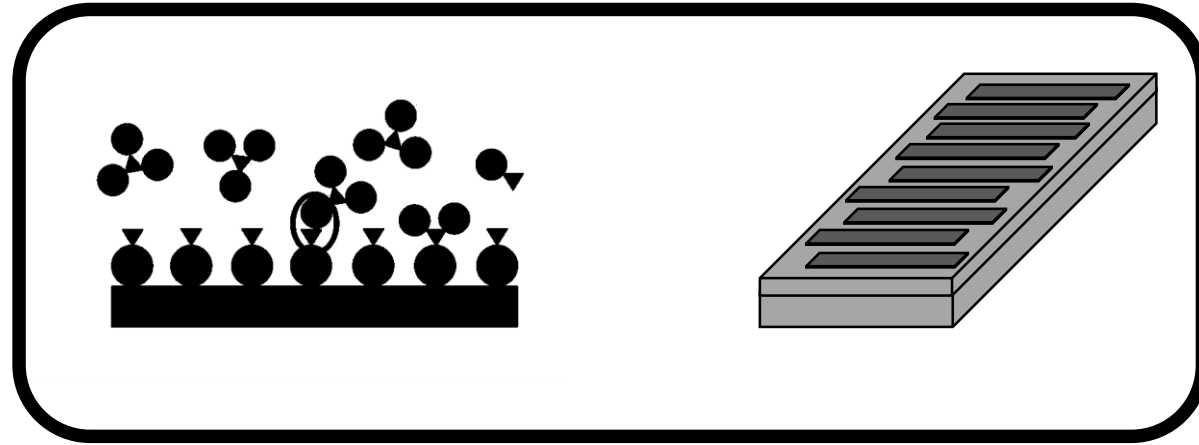


**Collaborator:**  
Prof. Aitor Mugarza  
**FunNanoSurf:**  
Dr. Daniel Herrera



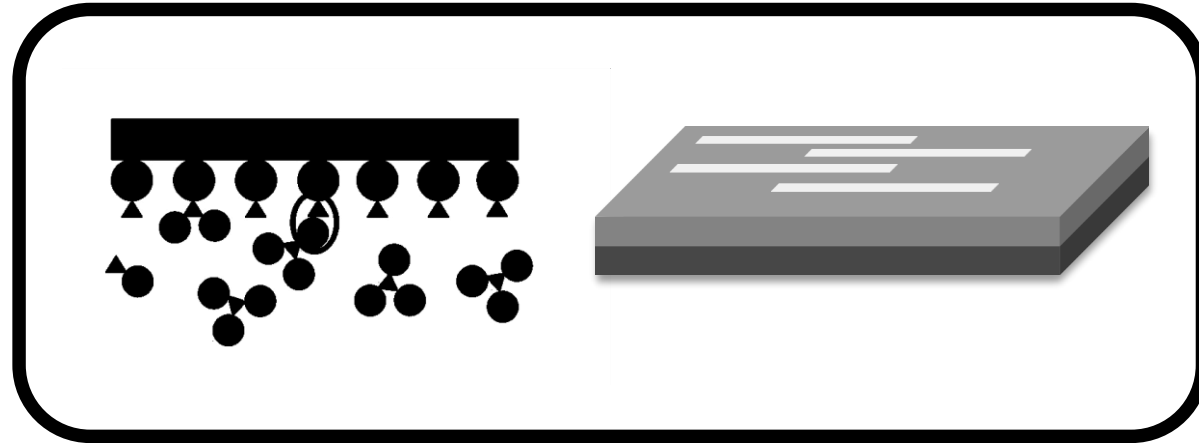
Goslinski *et al.*, *Inorganic Chemistry Communications*, **2012**, 20, 13; Tarakanov *et al.* *Dalton Transactions*, **2018**, 47, 14169.  
Abd El-Rahman *et al.*, *Biological and Pharmaceutical Bulletin*, **2018**, 41, 1071; Ahmed *et al.*, *Chemical Biology & Drug Design*, **2018**, 91, 338.

# Guidelines



Deposition methods & Measurements

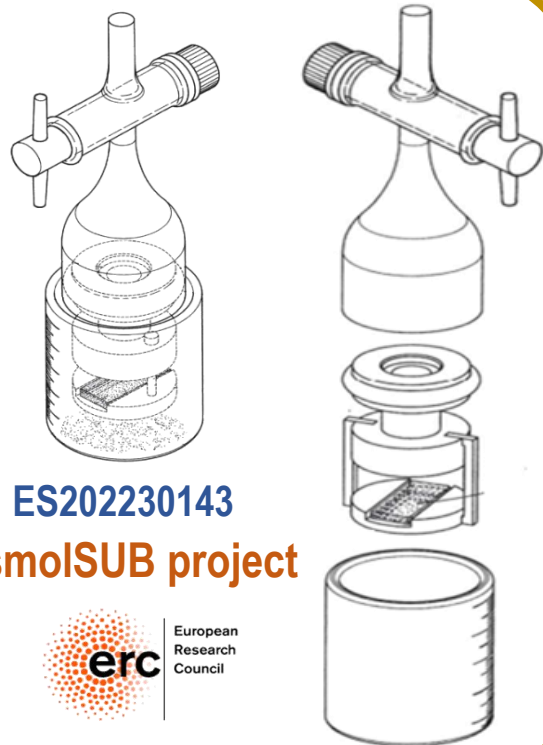
# Guidelines



Sublimation & Electronic studies



# Sublimation: CCMoids on surfaces



Surface

ES202230143  
smolSUB project



**FunNanoSurf:**  
Dr. Daniel Herrera  
Dr. Rossella Zaffino  
Gerard Felipo-Esteve

## Parameters

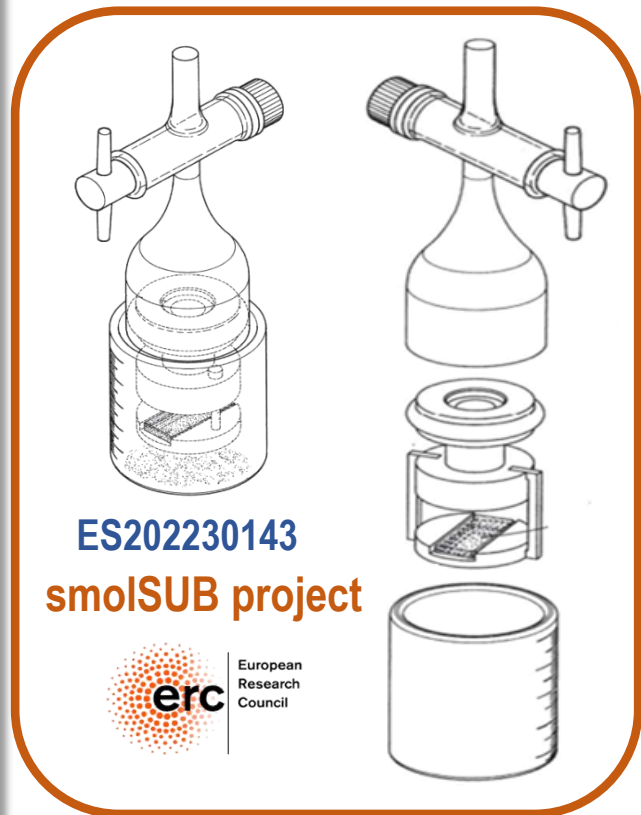
- d (Distance substrate-material)
- M (grams of sample)
- P (pressure in mbar)
- T (sublimation temperature)
- t (sublimation time)



Molecular material



# Sublimation: CCMoids on surfaces

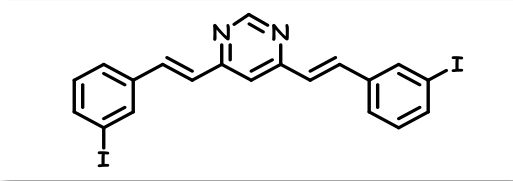


Surface

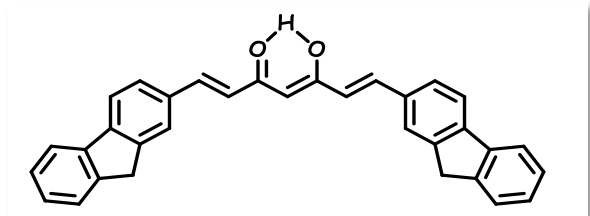
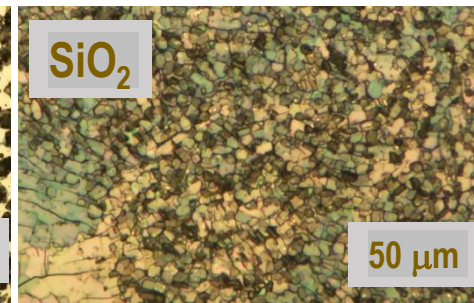
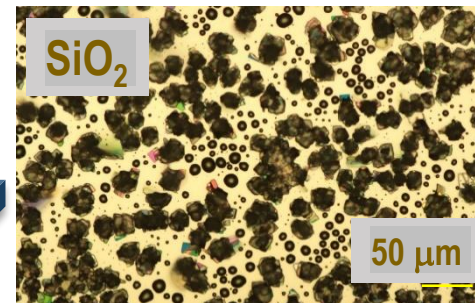


Molecular material

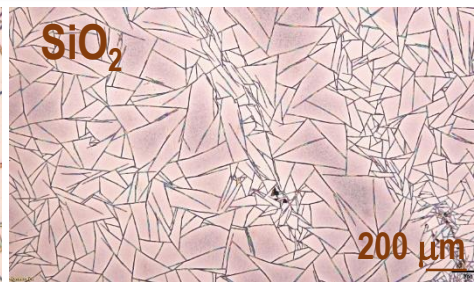
- Parameters**
- d (Distance substrate-material)
  - M (grams of sample)
  - P (pressure in mbar)
  - T (sublimation temperature)
  - t (sublimation time)



d = 1.5 cm  
 M = 5.1 mg  
 P = 9.0 mbar  
 T = 200 °C  
 t = 2.15 h



d = 1.5 cm  
 M = 3.0 mg  
 P = 8.0 mbar  
 T = 248 °C  
 t = 2.15 h



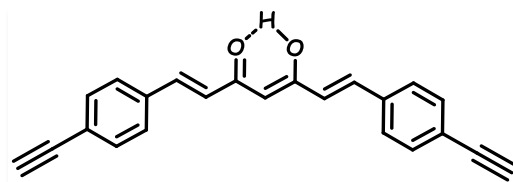
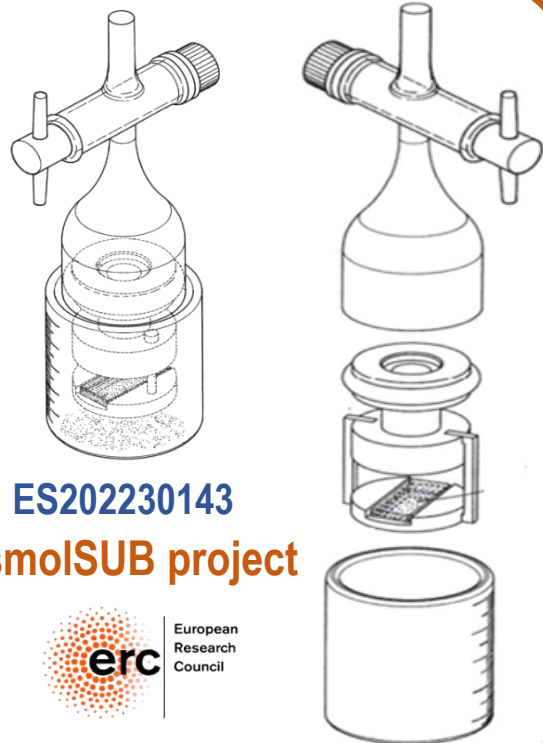
ES202230143  
 smolSUB project



**FunNanoSurf:**  
 Dr. Daniel Herrera  
 Dr. Rossella Zaffino  
 Gerard Felipo-Esteve



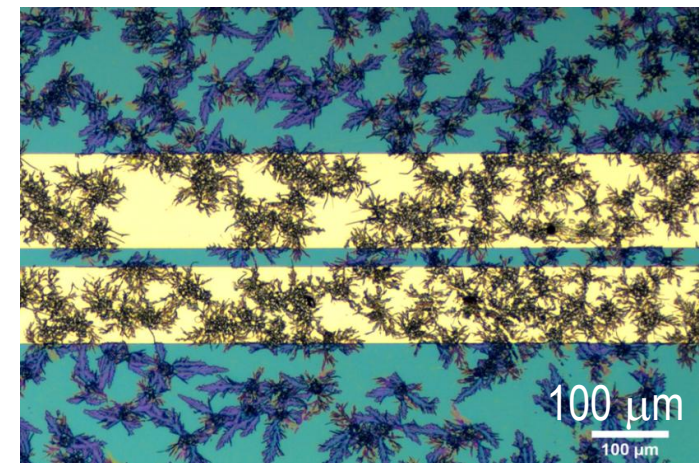
# Sublimation: CCMoids on devices



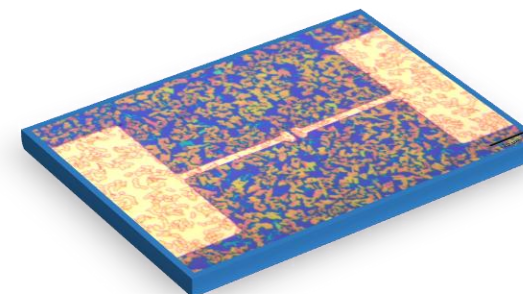
Pre-patterned device



Molecular material



$\sigma > 2.7 \times 10^{-7} \text{ Scm}$  (Ambient conditions)



OED ready for testing

ES202230143  
smoSUB project

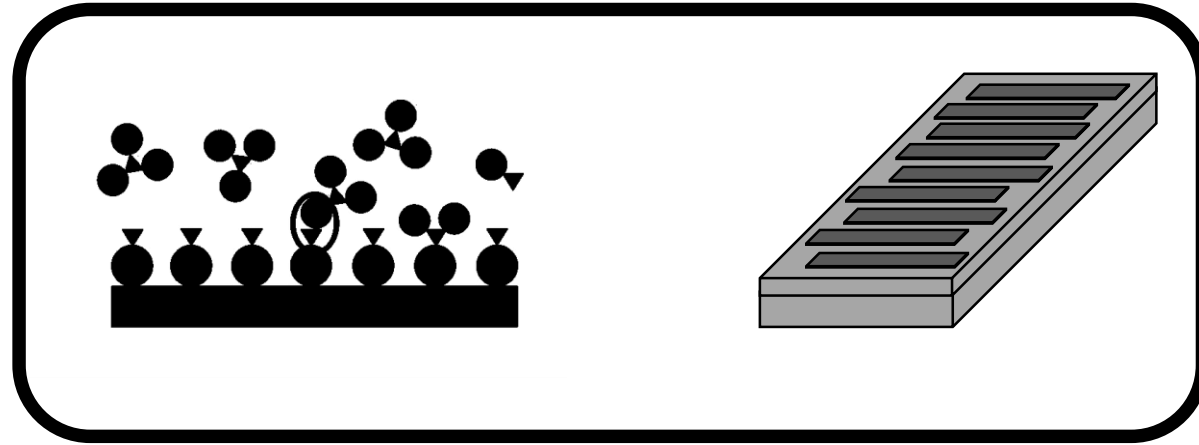


**FunNanoSurf:**  
Dr. Daniel Herrera  
Dr. Rossella Zaffino  
Gerard Felipo-Esteve

## Parameters

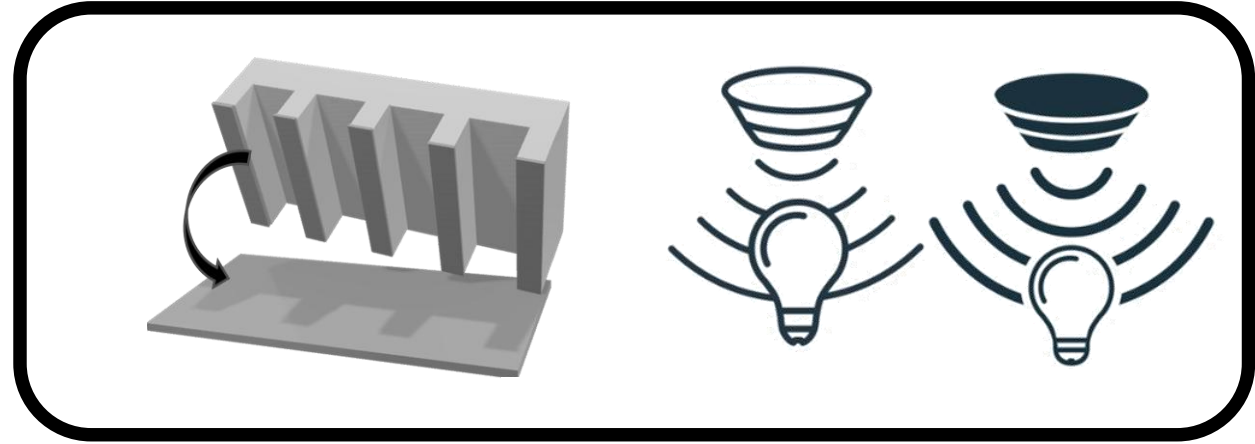
- d (Distance substrate-material)
- M (grams of sample)
- P (pressure in mbar)
- T (sublimation temperature)
- t (sublimation time)

# Guidelines

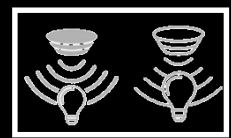


Deposition methods & Measurements

# Guidelines



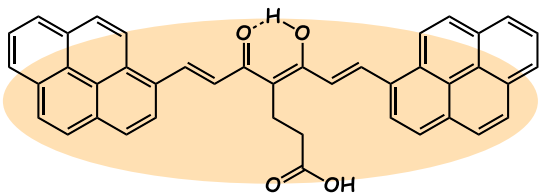
$\mu$ -contact printing & Sensing



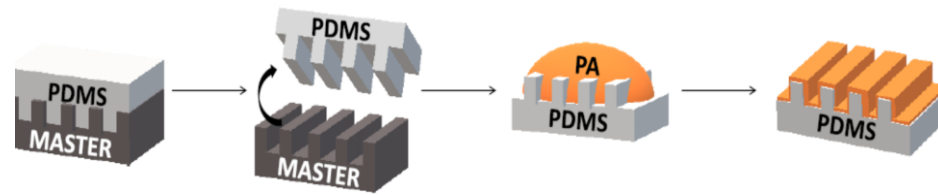
# Soft contact: CCMoids on glass

Micro-contact printing ( $\mu$ CP)  
PDMS stamp  
Functionalized Surface

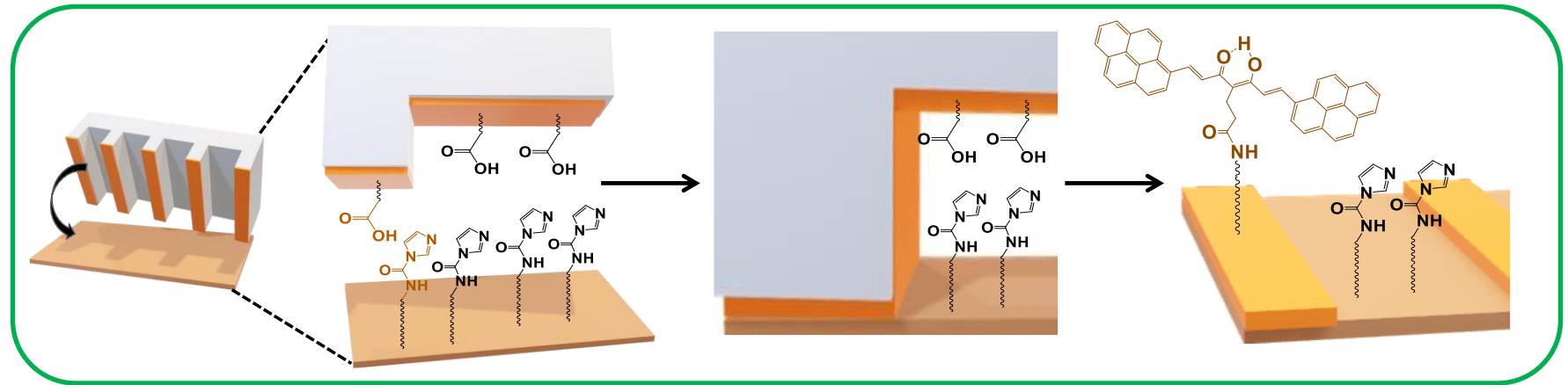
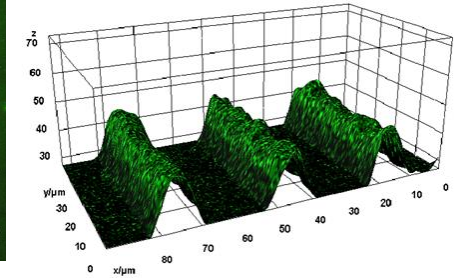
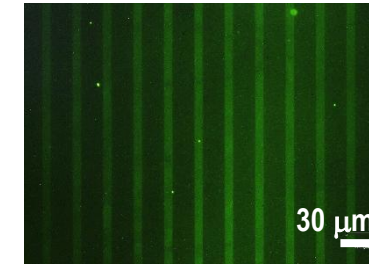
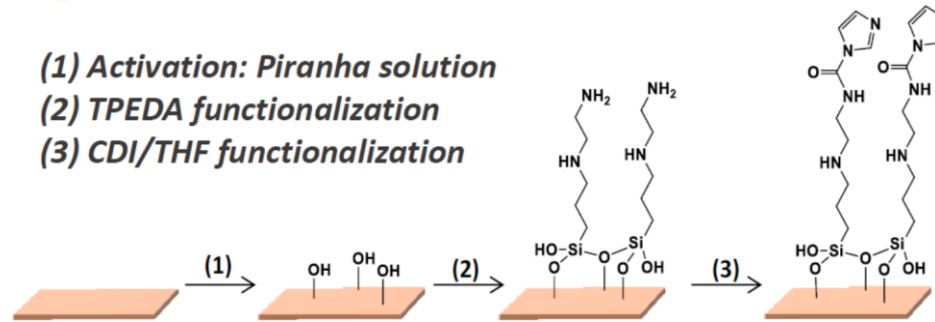
CCMoid molecule



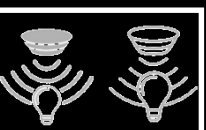
FunNanoSurf:  
Raquel Gimeno-Muñoz



- (1) Activation: Piranha solution
- (2) TPEDA functionalization
- (3) CDI/THF functionalization

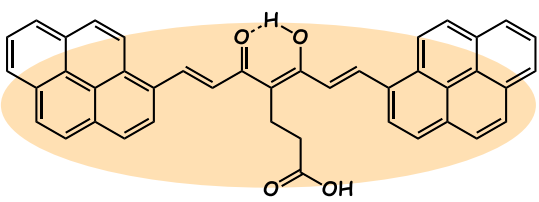


# Characterization studies of CCMoids on glass



Micro-contact printing ( $\mu$ CP)  
PDMS stamp  
Functionalized Surface

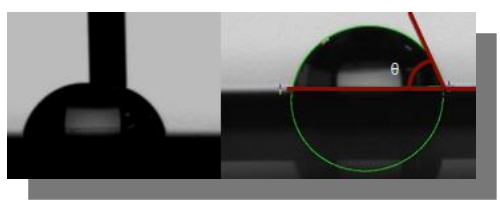
CCMoid molecule



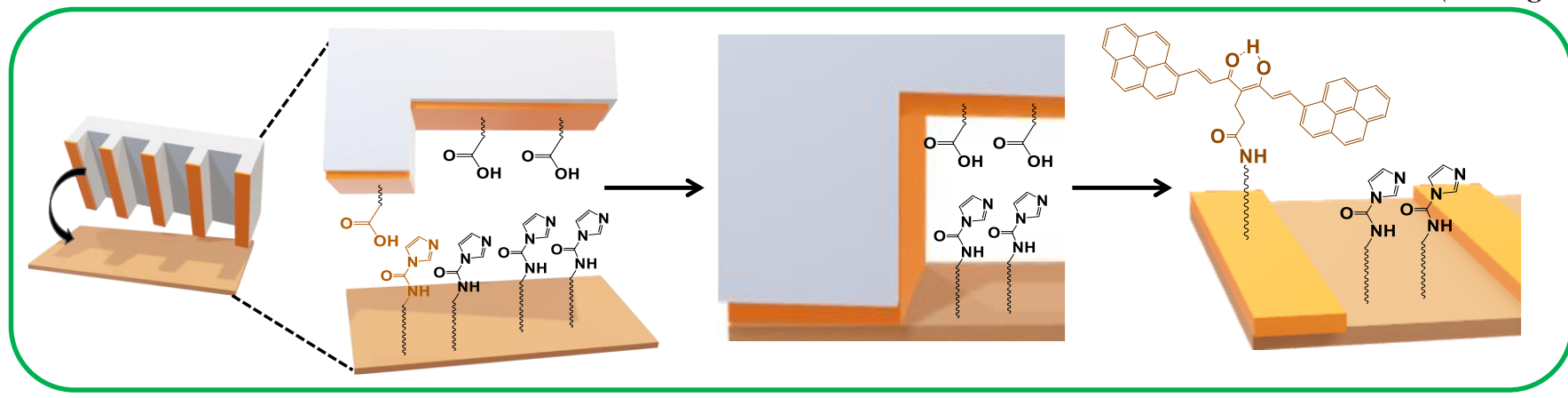
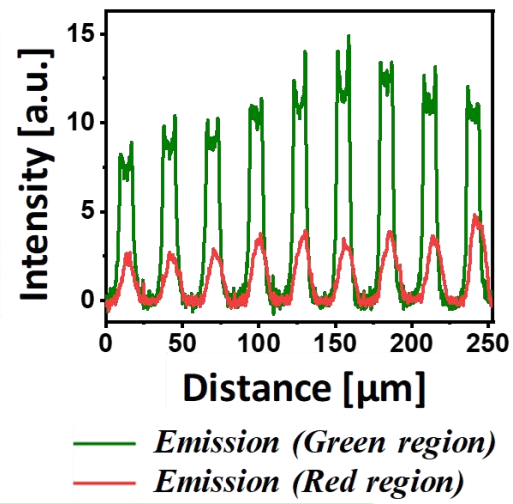
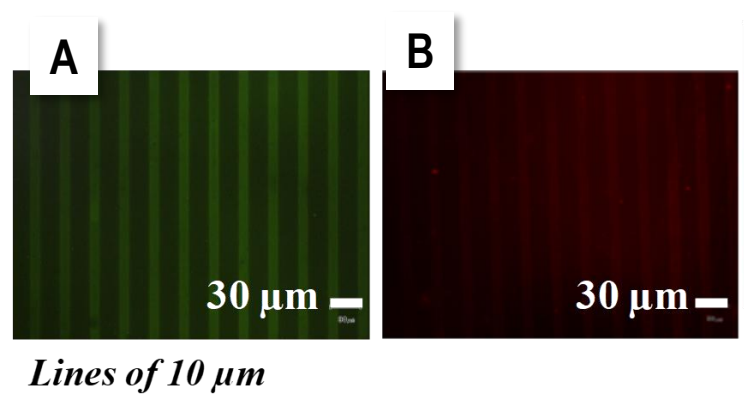
Lines of 5 and 10  $\mu$ m  
Fluorescence microscopy  
Green emission

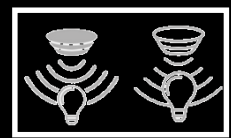
## Characterization:

- Contact angle measurements
- Fluorescence microscopy
- Confocal microscopy
- XPS measurements



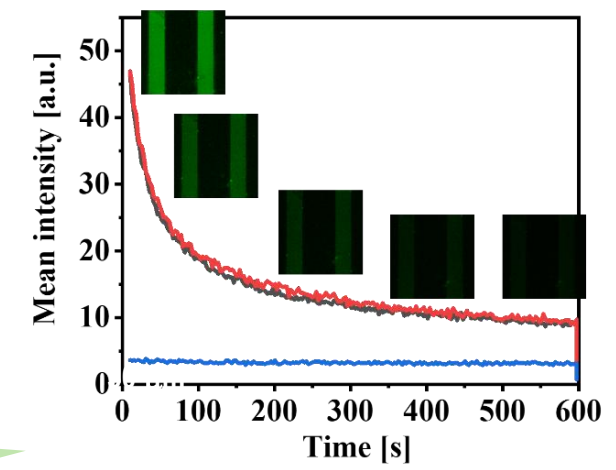
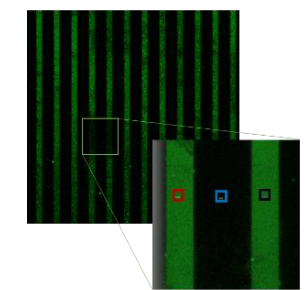
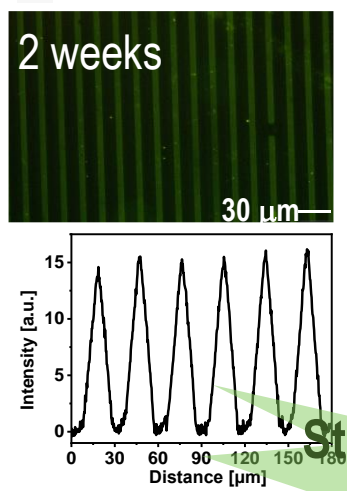
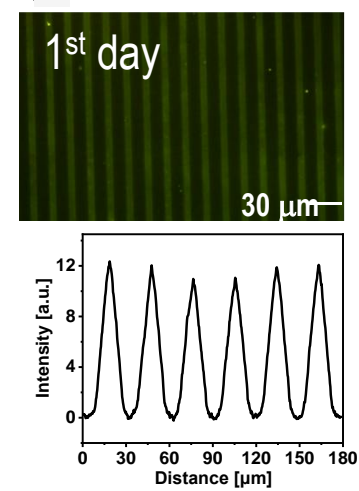
A) EXC.FILTER: ( $450 \text{ nm} \leq \lambda_{\text{ex}} \leq 480 \text{ nm}$ ) EM. FILTER :  $\lambda_{\text{em}} \geq 515 \text{ nm}$   
B) EXC. FILTER: ( $510 \text{ nm} \leq \lambda_{\text{ex}} \leq 550 \text{ nm}$ ) EM. FILTER:  $\lambda_{\text{em}} \geq 590 \text{ nm}$



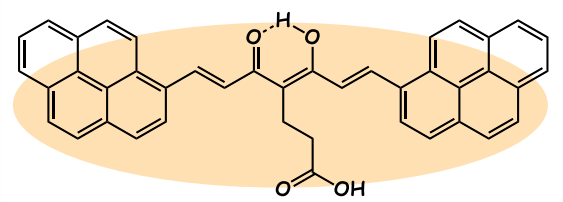


# Studies of stability of CCMoids on glass

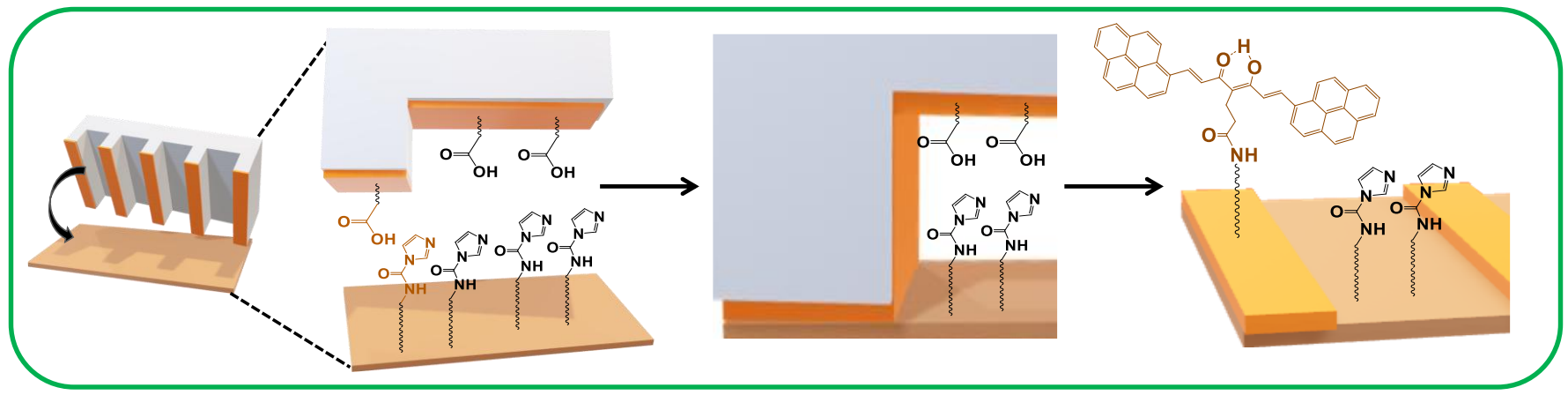
Micro-contact printing ( $\mu$ CP)  
PDMS stamp  
Functionalized Surface  
**CCMoid molecule**

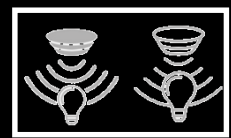


Stable surfaces for  
more than two  
weeks



Lines of 5 and 10  $\mu$ m  
Fluorescence microscopy  
**Green emission**

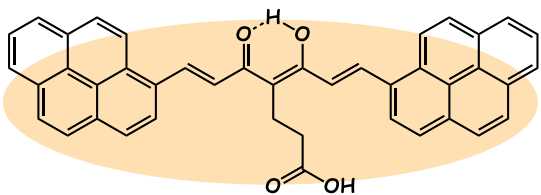




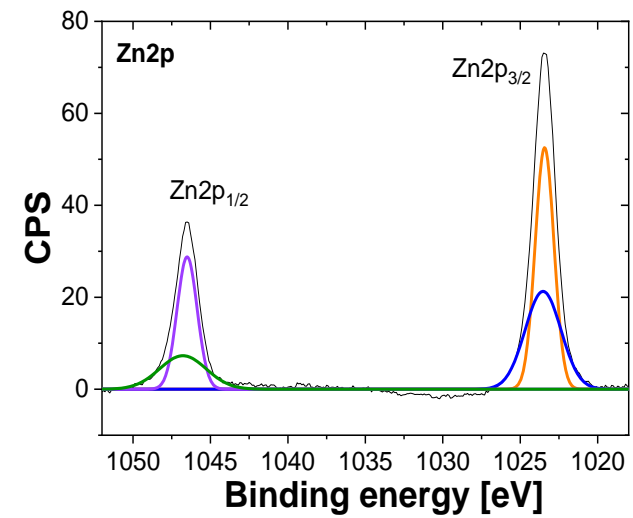
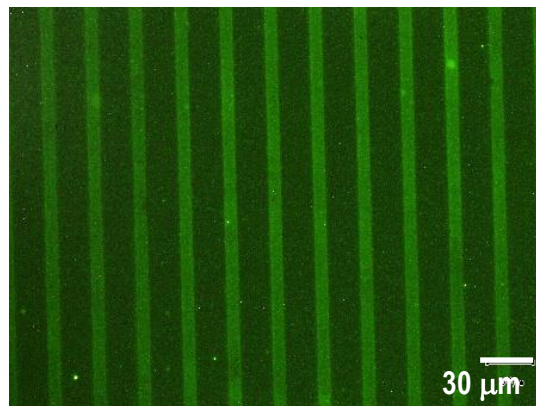
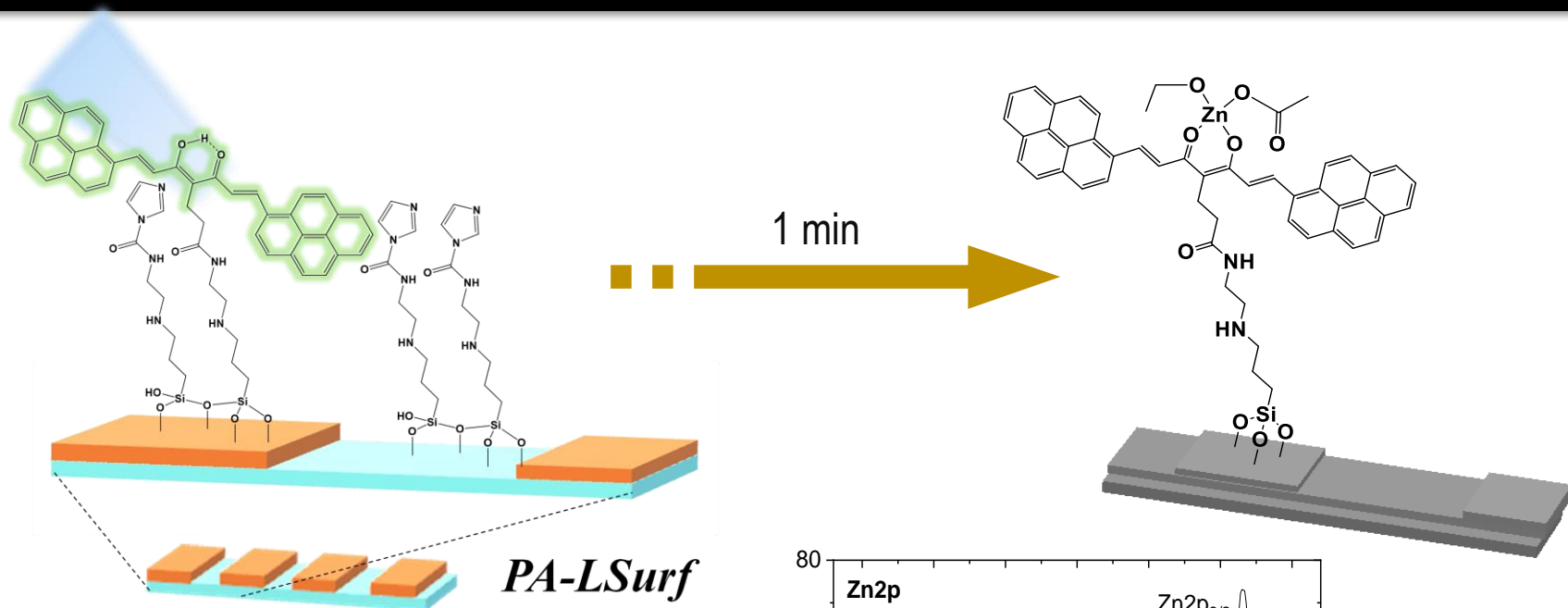
# Responsive substrates – Zn(II)

Micro-contact printing ( $\mu$ CP)  
PDMS stamp  
Functionalized Surface

CCMoid molecule



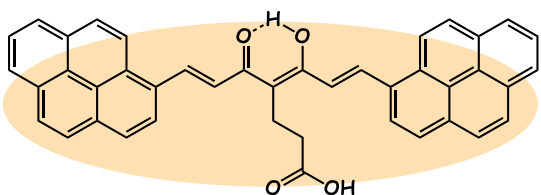
Lines of 5 and 10  $\mu$ m  
Fluorescence microscopy  
Green emission



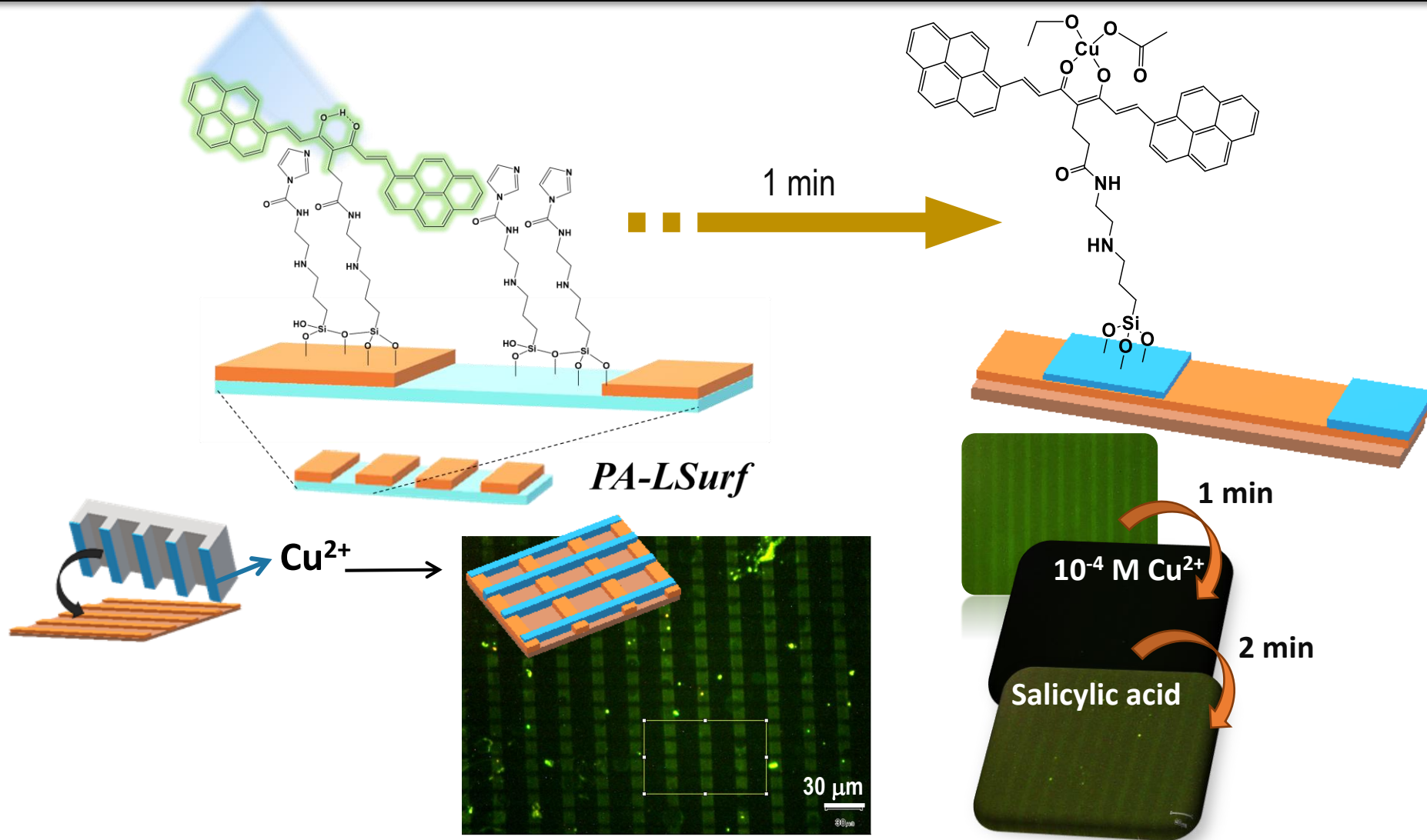
# Responsive substrates – Cu(II)

Micro-contact printing ( $\mu$ CP)  
PDMS stamp  
Functionalized Surface

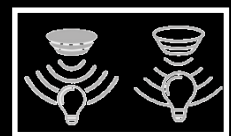
CCMoid molecule



Lines of 5 and 10  $\mu$ m  
Fluorescence microscopy  
Green emission



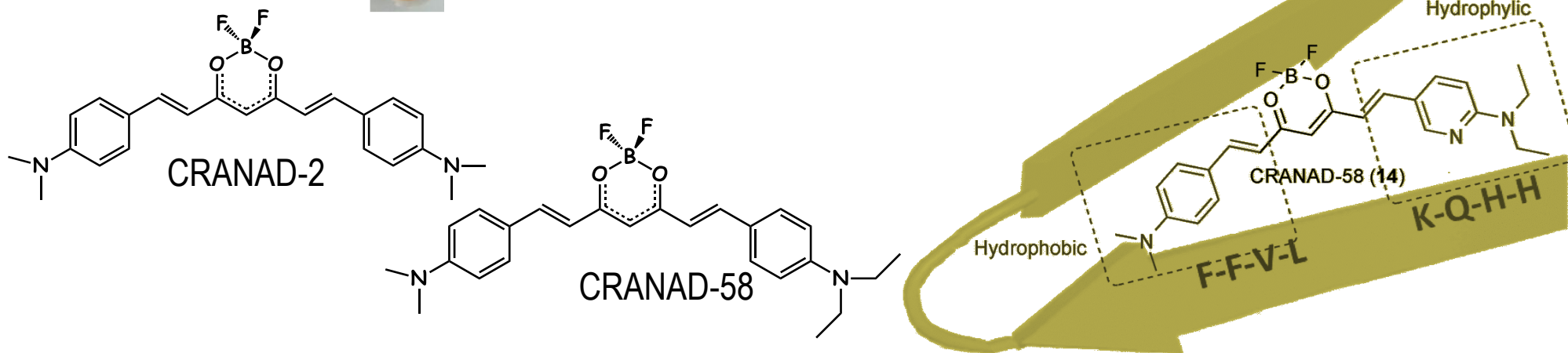
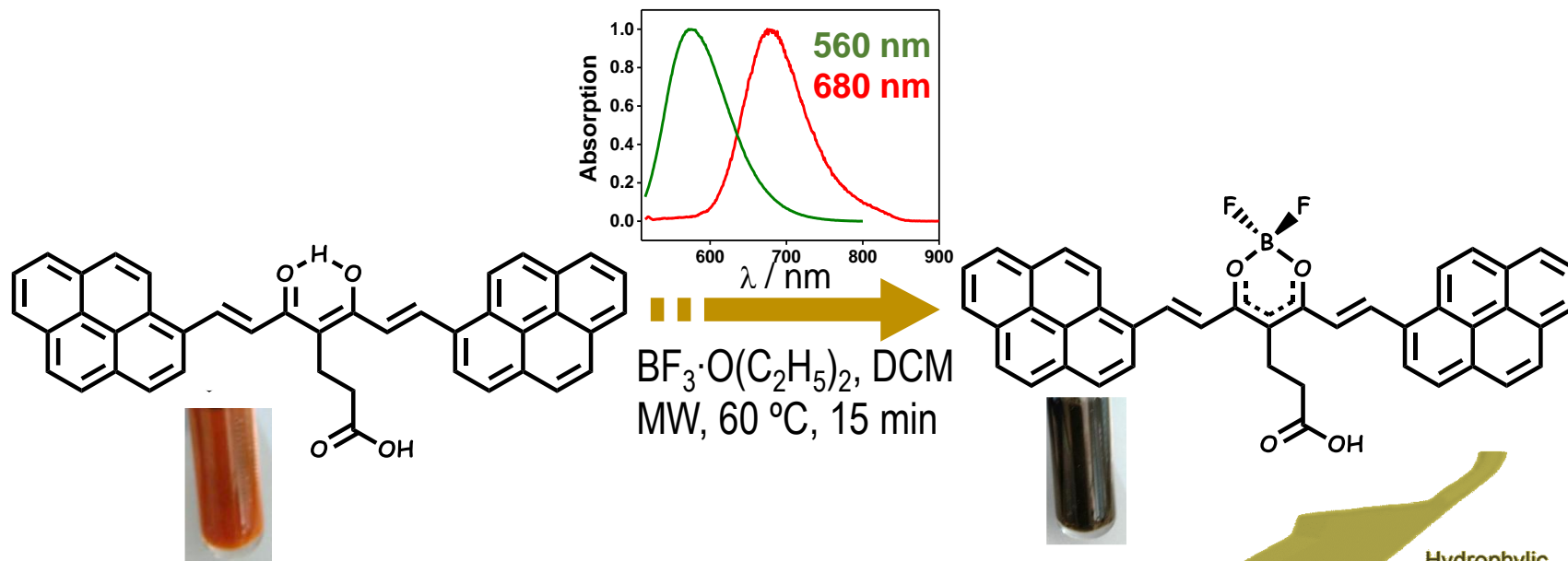
Work in progress

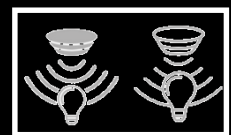


# In solution: CCMoids and $\text{BF}_3$

$\text{BF}_3$  is a toxic gas with global demand in industry

$\text{BF}_2$ -CCMoids present relevant shifts of their absorbing bands





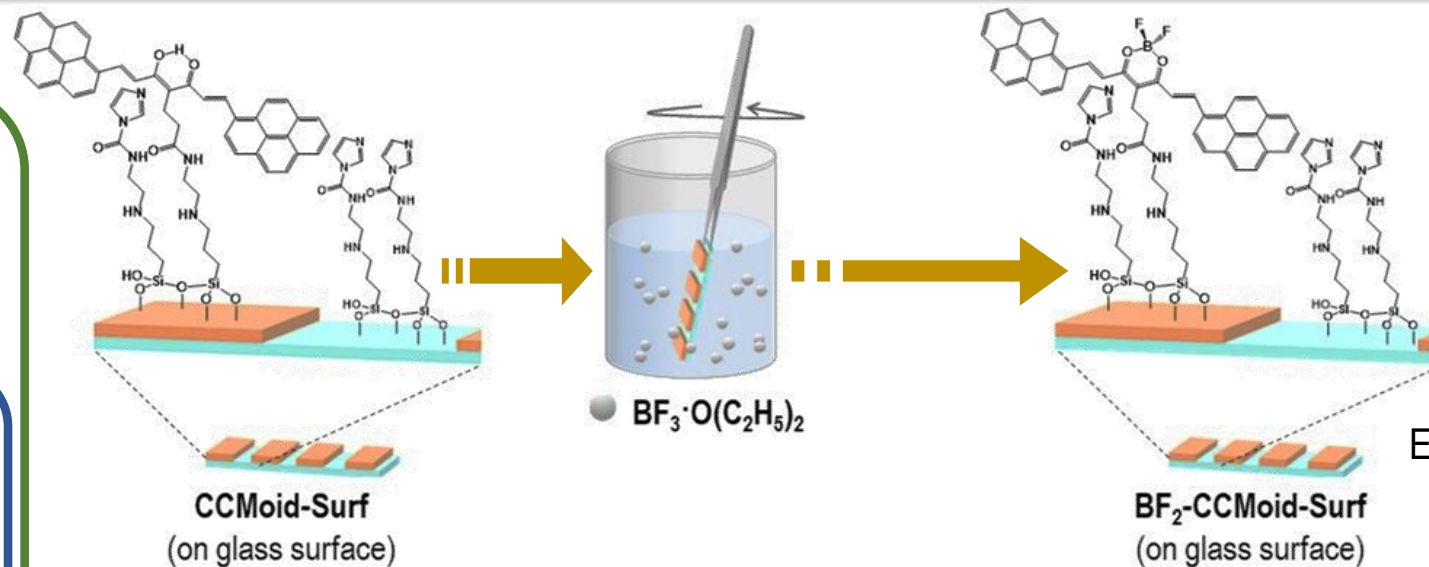
# Detection of $\text{BF}_3$

## CCMoid on glass

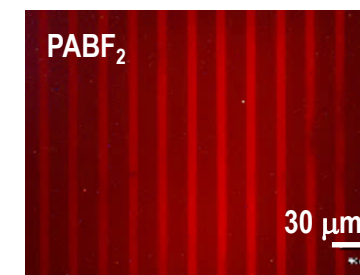
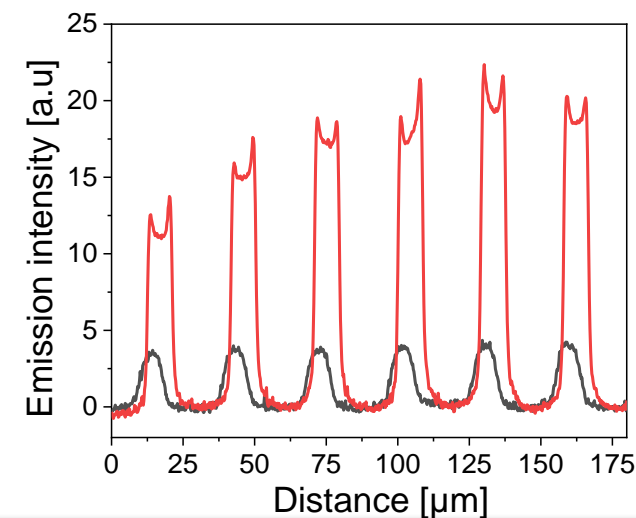
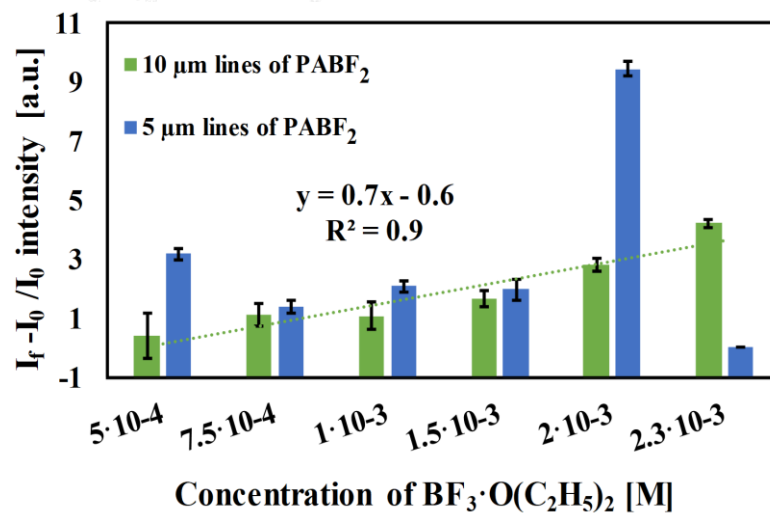
Coordination with  $-\text{BF}_2$   
red emission

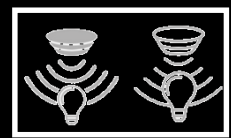
Lines of 5 and 10  $\mu\text{m}$

FunNanoSurf:  
Raquel Gimeno-Muñoz



EXC. FILTER: ( $510 \text{ nm} \leq \lambda_{\text{ex}} \leq 550 \text{ nm}$ )  
EM. FILTER:  $\lambda_{\text{em}} \geq 590 \text{ nm}$





# ON-OFF-ON system

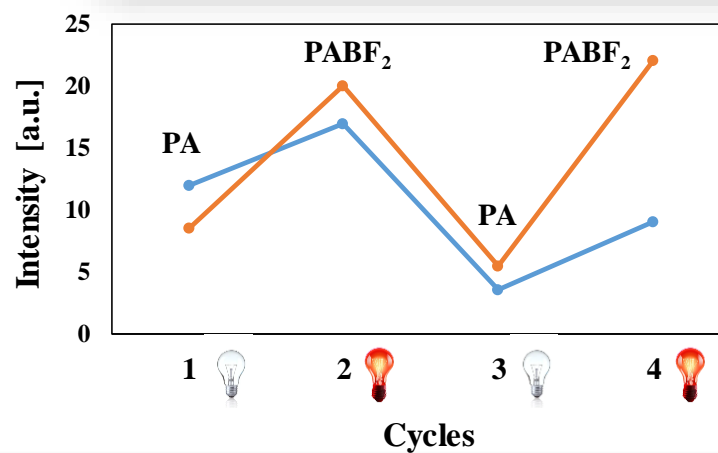
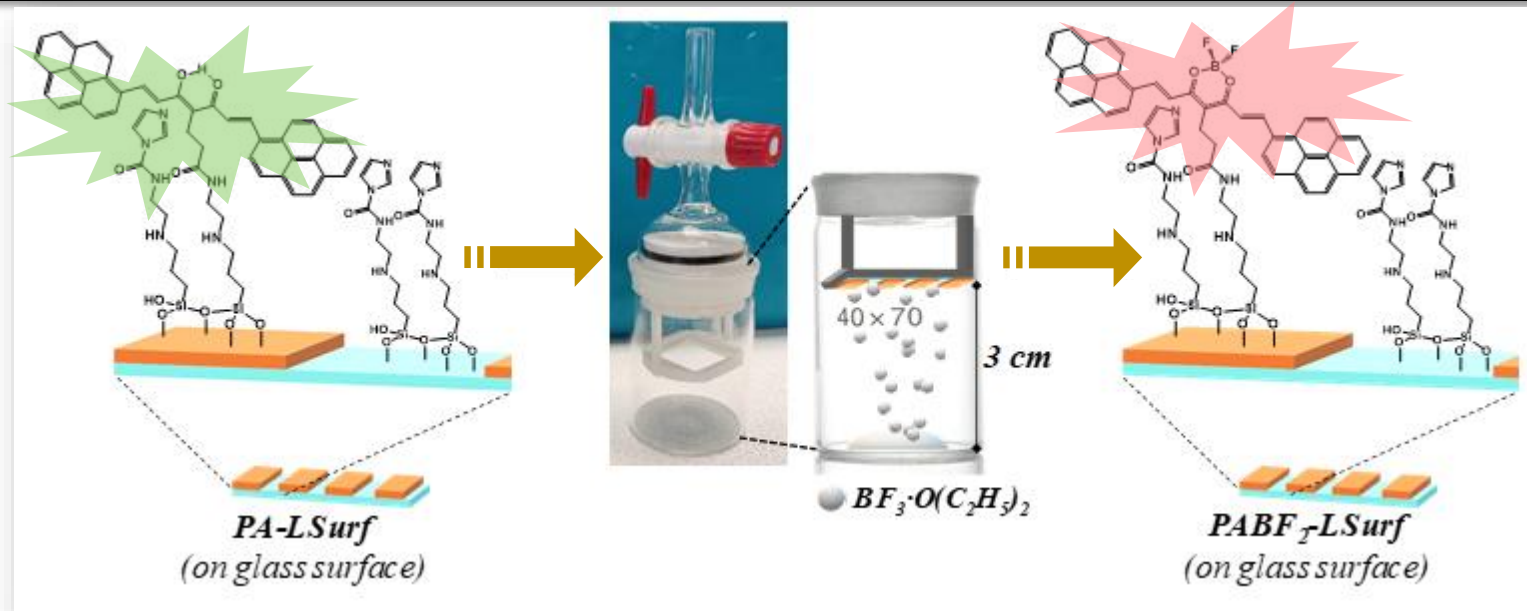
## CCMoid on glass

Coordination with  $-\text{BF}_2$   
red emission

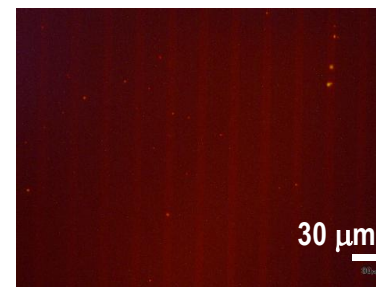
Lines of 5 and 10  $\mu\text{m}$

— Basic solution  
—  $\text{H}_2\text{O}$

FunNanoSurf:  
Raquel Gimeno-Muñoz

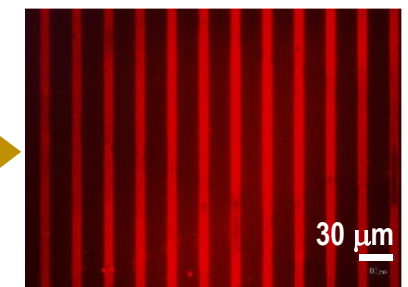


EXC. FILTER: ( $510 \text{ nm} \leq \lambda_{\text{ex}} \leq 550 \text{ nm}$ )  
EM. FILTER:  $\lambda_{\text{em}} \geq 590 \text{ nm}$



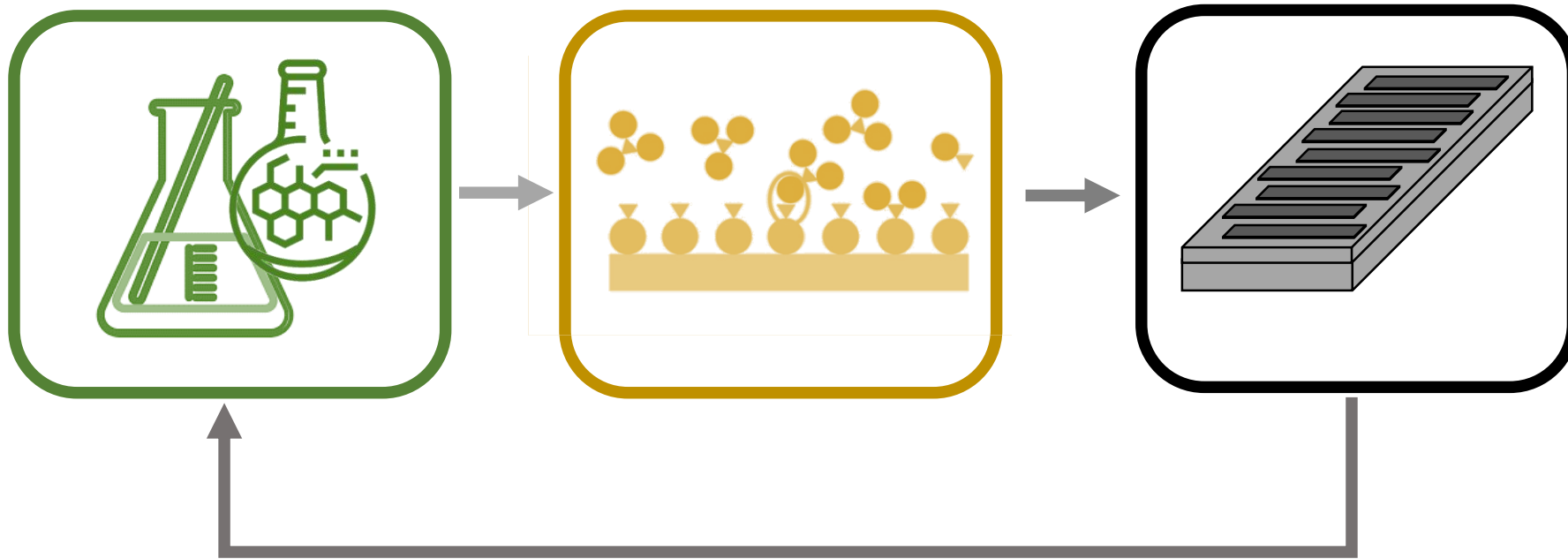
**PA-LSurf**

$\text{BF}_3 \cdot \text{O}(\text{C}_2\text{H}_5)_2$   
2 min



**PABF<sub>2</sub>-LSurf**

# Summary



## Substrates

New molecular formulations having asymmetric CCMoids that will assist the attachment of the molecules on different substrates.

Solubility and molecular extension studies

### Collaborators:

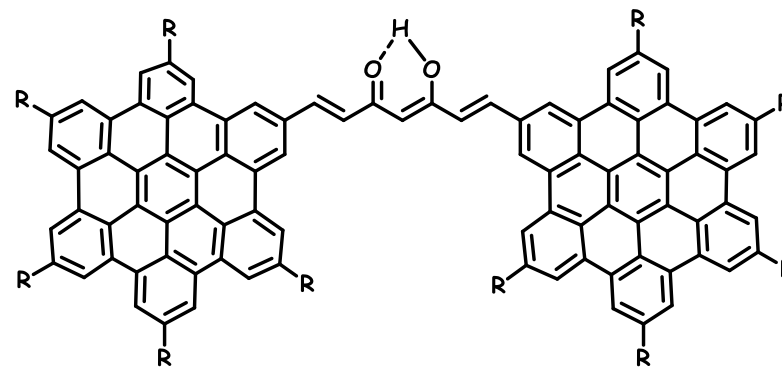
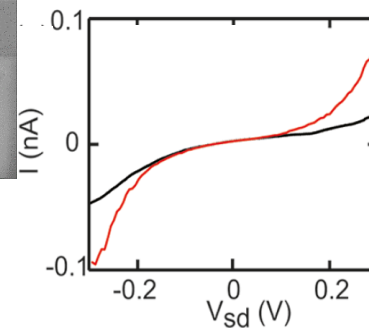
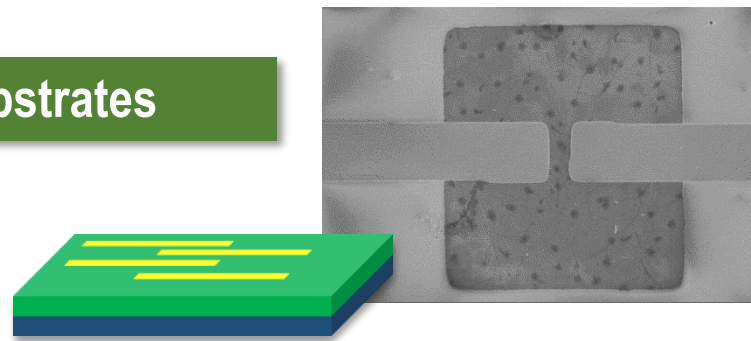
Prof. Eliseo Ruiz

Prof. Diego Peña

### FunNanoSurf

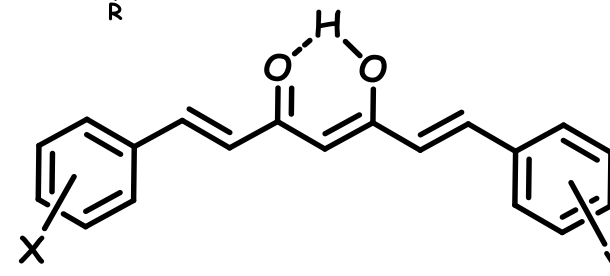
Dr. Daniel Herrera

Dr. Rossella Zaffino



## Nanographene-based CCMoids

## Asymmetric CCMoids



# Collaborations

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Prof. Josep Puigmartí-Luis  
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Dr. Guillem Aromí  
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## University of Wageningen

Prof. Aldrik Welders

## University of Texas (el Paso)

Prof. Luis Echegoyen

## KU Leuven

Prof. Xavier Casadevall i Solvas

## Universidad Miguel Hernández de Elche

Prof. Ángela Sastre-Santos

# FUNctional NANOmateriAls & SURFaces



724981, Tmol4TRANS  
101138186, smolSUB



PID2023-151929NB-I00,  
**AsyCCMoidsACT** MICIU/AEI  
/10.13039/501100011033 & FEDER, UE



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**Dr. Daniel Herrera**

**Dr. Sara Battista**

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**Carlos Cascales-Guerrero**

**Teresa Cardona-Lamarca**

**Joseline Iribarra-Araya**



## Master Student

**Gerard Felipo-Esteve**



## IT Project Manager

**Dr. Coral Herranz-Lancho**

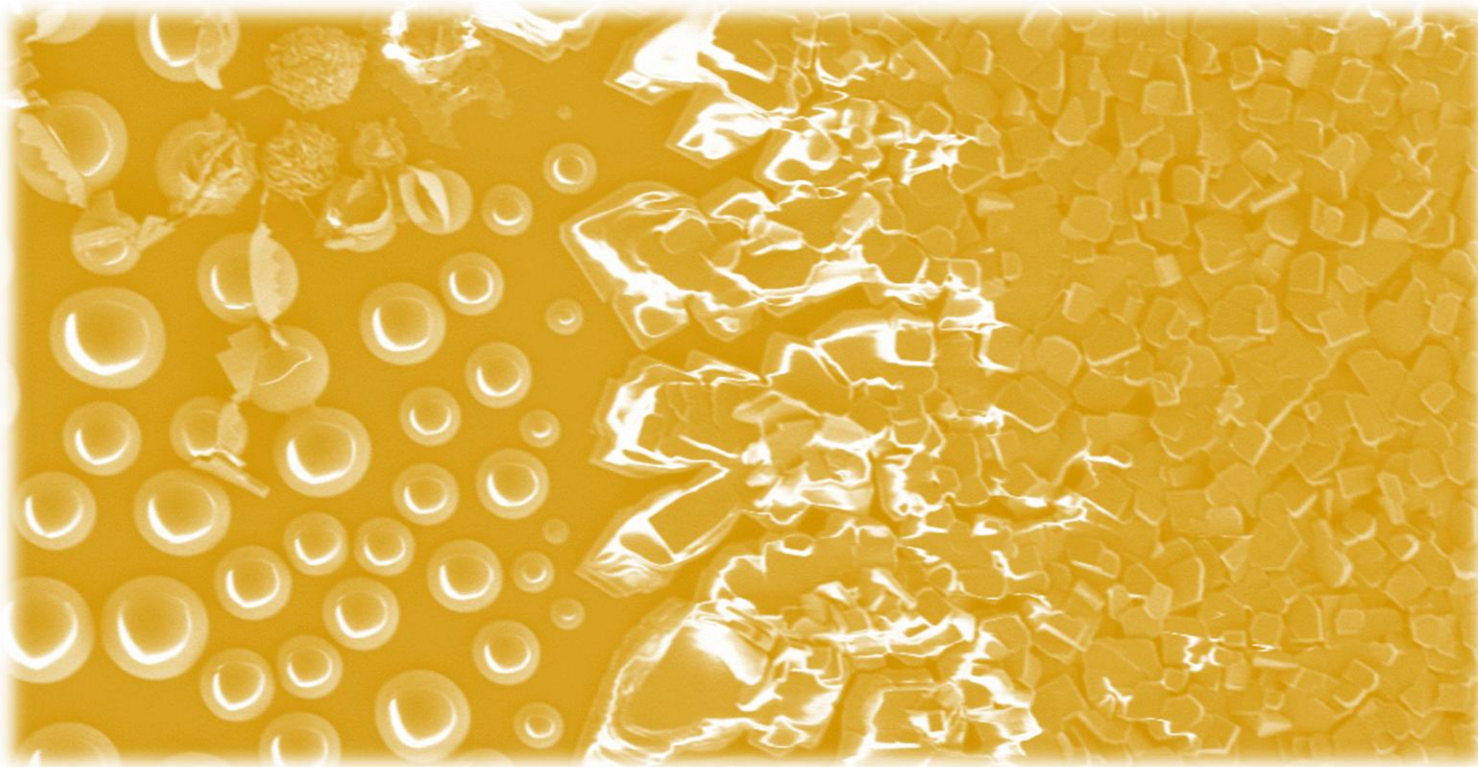


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Thank you for your  
attention