# #ESNoINa 2023

### 16<sup>th</sup> European School on Molecular Nanoscience

#esmolna2023

May 7 <sup>th</sup> to 11<sup>th</sup> 2023.

San Lorenzo de El Escorial, Madrid. (Spain)



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**Organized by:** 







**Sponsors:** 











### The School #ESMolNa2023

The 16th European School on Molecular Nanoscience (ESMol-Na2023) intends to provide a suitable framework to show and extensively discuss the state-of-the-art in these multidisciplinary areas. Lectures are aimed at the post-graduate level as they will be presented to an audience primarily formed by post-graduate, PhD students and postdoctoral fellows. In fact, the School will be the last part of an intensive Advanced Course of three weeks organized in the frame of a Master in Molecular Nanoscience and Nanotechnology. This meeting also intends to be a forum where the active European scientific groups working in these areas will have the opportunity to meet and informally discuss with the younger generations.

# Organizers & Committee



#### Organizers

The school is organized by the Instituto de Ciencia Molecular (ICMol) of the Universitat de València and the Universidad Autónoma de Madrid.

#### Committee



**Eugenio Coronado** 

#### Chair

European Institute of Molecular Magnetism (EIMM) & ICMol -Universitat de València, Spain



Giovanni Bottari <sup>Chair</sup>

Universidad Autónoma de Madrid, Spain



**Tomás Torres** 

Universidad Autónoma de Madrid, Spain

#### **Conference Secretary:**

Paco Escrig Escrig

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The talks will be held at the Real Centro Universitario María Cristina in San Lorenzo de El Escorial (Madrid, Spain) where attendants will be also hosted and meals will be served.

## Invited Speakers

### Abstracts





Guillem AROMÍ Univ. of Barcelona (ES)





Johannes BARTH





Lapo BOGANI Univ. of Oxford (UK)





Davide BONIFAZI

Univ. of Vienna (AT)





David ÉCIJA IMDEA Nanoscience (ES)





Sandrine HEUTZ Imperial College London (UK)





Sebastian LOTH Univ. of Stuttgart (DE)





**Fernando LUIS** Univ. of Zaragoza (ES)





Rodolfo MIRANDA





Tatjana PARAC-VOGT KU Leuven (BE)





Fernando MARTIN IMDEA Nanoscience - UAM (ES)





María VARELA Complutense Univ. of Madrid (ES)



#### **Structure & Topics**

**General invited lectures (50 min + 10 min discussion):** This part will deal with the essential aspects of Molecular Nanoscience on the topics:

Supramolecular Chemistry in Nanoscience / Concepts, materials and applications of Molecular Electronics / Single-Molecule Electronics / Molecular Nanomagnetism / Molecule-based Spintronics

**Specialized invited lectures (25 min + 5 min discussion):** In this part, short tutorial lectures showing some relevant scientific advances in the above topics will be presented by the most representative European research groups active in Molecular Nanoscience.

Oral communications (8 min + 2 min discussion) or Flash presentations (4 min + 1 min discussion): With the aim of encouraging discussion and communication among all the participants, the students will have the opportunity to present short communications about their research results, including those that, although incomplete, can promote debate.

# Program

May/2023	Sunday 7 <sup>th</sup>	Monday 8 <sup>th</sup>	Tuesday 9 <sup>th</sup>	Wednesday 10 <sup>th</sup>	Thursday 11 <sup>th</sup>	
9:00-9:30		C. Houtz	M. Marala		C. Aromí	9:00-9:30
9:30-10:00		5. Heulz	w. vareia	T. Parac-vogi	G. Afomi	9:30-10:00
10:00-10:30		Y. Manassen	M. Ince	I Dorth	E Luio	10:00-10:30
10:30-11:00		G. Gramse	M.C. Ruiz	J. Darth	F. Luis	10:30-11:00
11:00-11:30		Coffee break	Coffee break	Coffee break	Coffee break	11:00-11:30
11:30-12:00		J. Soriano	D. Pinkowicz	M.A. Herrero	L. Escalera	11:30-12:00
12:00-12:30		R. Sanchis	S. Triki	R. Calvo		12:00-12:30
12:30-13:00		N. Aliaga	K. Boukheddaden	N. Pascual	M. Briganti	12:30-13:00
13:00-13:30			E. Cánovas			13:00-13:30
13:30-14:00						13:30-14:00
14:00-14:30	)	LUNCH	LUNCH	LUNCH	LUNCH	14:00-14:30
14:30-15:00						14:30-15:00
15:00-15:30						15:00-15:30
15:30-16:00				Maitte El Essevial		15:30-16:00
16:00-16:30	Pagiotration			VISIT TO ELESCORIAL Monastery		16:00-16:36
16:30-17:00	negistration	D. Popifozzi	L Pogoni	Monastery	S. Loth	16:30-17:00
17:00-17:30	Walaama	D. DUIIIazzi	L. Doyani			17:00-17:30
17:30-18:00	weicome	C. Romero	Flash presentation	E Martín	Flash presentation	17:30-18:00
18:00-18:30	P. Miranda	Coffee break	Coffee break	F. Martin	Coffee break	18:00-18:30
18:30-19:00	n. Milianua	Flash		Flash		18:30-19:00
19:00-19:30	D Ésile	Presentations	& Oral	Presentations	& Oral Communications	19:00-19:30
19:30-20:00	D. Ecija	& Oral	Communications	& Oral	Communications	19:30-20:00
20:00-20-30	Popontion	Communications		Communications	Closing	20:00-20-30
20:30-21:00	песерион					20:30-21:00
21:00	DINNER	DINNER	DINNER	DINNER	COCKTAIL DINNER	21:00

08h00	SUNDAY 7 <sup>th</sup>	
16h00	Registration	
17h00	Eugenio CORONADO- ICMol- Univ. Valencia (ES)	Welcome. Introduction to Molecular Nanoscience
18h00	Rodolfo MIRANDA- IMDEA Nanoscience - UAM (ES)	Magnetism in Flatland
19h00	David ÉCIJA- IMDEA Nanoscience (ES)	On-surface synthesis
20h00	Reception cocktail	
21h00	Dinner	
08h00	MONDAY 8 <sup>th</sup>	
09h00	Sandrine HEUTZ- Imperial College London (UK)	Molecular spins: a tool for nanostructure characterisation and technology
10h00	Yishay MANASSEN- Ben Gurion Univ. (IL)	Signal atom or molecule magnetic resonance - both ESR and NMR with the scanning tunneling microscopy
10h30	Georg GRAMSE- Johannes Kepler Univ. (AT)	Electrodynamic microscopy methods for nanoscale characterization of functional materials
11h00	Coffee break	
11h30	Joaquín SORIANO LOPEZ- ICMol- Univ. València (ES)	Water as Energy Vector. Tuning the Water Oxidation Catalytic Activity of Polyoxometalates via Molecular Engineering
12h00	Roger SANCHIS GUAL- ETH Zurich (CH)	Fabrication strategies for soft biocompatible microrobots with functional capabilities
12h30	Nuria ALIAGA-ALCALDE- ICREA-ICMAB/CSIC (ES)	Compilation of studies on curcuminoids on two/three-terminal devices and surfaces
13h30	Lunch	
16h30	Davide BONIFAZI- Univ. Vienna (AT)	Tailoring molecular materials for printed electronics
17h30	Carlos ROMERO NIETO- Univ. Castilla-La Mancha (ES)	Phosphorus heterocycles as unique and versatile tools to develop multifunctional materials
18h00	Coffee break	
18h30	Gonzalo ABELLAN DUMONT- Univ. Autonoma Madrid (ES)	Chemical Transformations in COFs Driven by Light and pH Stimuli
	Javier MONTERO- Univ. Autónoma Madrid (ES)	Efficient and selective thiosemicarbazones for heavy metal sequestration from water. Aqueous Stability studies of their stable nontoxic materials.
	Violeta HURTADO- Univ. Valladolid (ES)	Encapsulation of quaternary ammonium salts modified nano-clays in electrospun fibers for sustainable removal of nitrates in water
	Esteban ZAMORA AMO- Univ. Autónoma Madrid (ES)	Exfoliation of non-laminar materials
Flash	Jonathan MACHÍ HERNÁNDEZ- ICMol- Univ. València (ES)	Heterometallic ZIF-8 analogues for light hydrocarbon separation
4'+1'	Mohammad Ali NASIRI - ICMol- Univ. València (ES)	Optimization of thermoelectric polymer-based generator embedded into a meta-surface absorber
	María MONDÉJAR LÓPEZ- Univ. Castilla-La Mancha (ES)	Polysaccharide film containing chitosan nanoparticles for food preservation
	Irene MATEO NAVARRO- Univ. Miguel Hernández (ES)	Synthesis and photophysical study of an azobenzene-containing oblique perylenediimide dyad
	Félix LIZALDE ARROYO- Univ. Valladolid (ES)	The future of cellular materials: High-Performance and Transparent Nanocellular Polymers
	Mercy Elena ÁRTEAGA VINZA- ICMol- Univ. València (ES)	Amphiphilic Scorpiand-like Complexes as Superoxide Dismutase Mimics.
Oral Comm 8'+2'	Enrique NIZA GONZÁLEZ- Univ. Castilla-La Mancha (ES)	Chitosan coated - biogenic silver nanoparticles from wheat residues as green antifungal and nanoprimig in wheat seeds
	Carlos D. PRADO SOCORRO- ICMol- Univ. València (ES)	Quantifying the Effects of Varying Polymer Electrolyte Concentrations on the Memristive Properties and Circuit Models of Organic Devices
	Juba SALHI- Sorbonne Univ	Ready-to-be-addressed oxo-clusters : individualized, periodically
	IPCM (FR) Alicia MOBCII LO MOBA- Univ	organized and disconnected from the substrate
	Castilla-La Mancha (ES)	Synthesis and characterization of self-healing materials
21h00	Dinner	

	TUESDAY 9 <sup>th</sup>			
09h00	María VARELA- Complutense Univ. Madrid (ES)	Electron microscopy of advanced materials		
10h00	Mine INCE- Tarsus Univ. (TR)	Photocatalytic Hydrogen Production by Phthalocyanine based Photocatalyst		
10h30	M. Carmen RUIZ DELGADO- Univ. Málaga (ES)	Understanding the electronic properties of organic conjugated materials from a joint experimental and theoretical approach		
11h00	Coffee break			
11h30	David PINKOWICZ- Jagiellonian Univ. (PL)	Photochemical approach to the design and synthesis of molecular photomagnets		
12h00	Smaïl TRIKI- Univ. Brest (FR)	Correlation between emission and mechanical properties in spin crossover composites		
12h30	Kamel BOUKHEDDADEN- Univ. Versailles- Saint Quentin (FR)	Imaging and modelling the Spatio-temporal Dynamics of First-Order Spin Transitions in Spin-Crossover Single Crystals		
13h00	Enrique CÁNOVAS- IMDEA Nanoscience (ES)	Non-contact electrical characterization of 2D MOFs and COFs by time resolved THz spectroscopy		
13h30	Lunch			
16h30	Lapo BOGANI- Univ. Oxford (UK)	A new wave of quantum carbon		
17h30	María Inmaculada GOMAR FERNÁNDEZ- ICMol- Univ. València (ES)	Close Space sublimation for development of efficient perovskite solar cells		
	Álvaro ROYO DE LARIOS- ICMol- Univ. València (ES)	Computational study of hydrogen-bonded organic frameworks based on tetrathiafulvalene building block and its selenium/tellurium analogues.		
<b>F</b> lash	Alex FARRANDO PEREZ- Univ. Alicante (ES)	Near-Infrared Lasing in Perylene-Based Linear Non-alternant Nanoribbons.		
Flash Pres. 4'+1'	Fernando DÉNIZ CORREA- Univ. La Laguna (ES)	New optical active doped perovskites based on ytterbium.		
	Mario FERNÁNDEZ DE LA FUENTE- Univ. Valladolid (ES)	Open-Cell Nanocellular Polymers: A Promising Solution for Green Insulation and Filtration		
	Garoé MEDINA- Univ. La Laguna (ES)	Structural and optical Characterization of new lanthanide doped perovskite type oxides		
18h00	Coffee break			
18h30	Pedro XIMENIS CAMPINS- Univ. València (ES)	Synthesis and self-assembly studies of π-conjugated dipyrrolidones		
Flash	Jose Alejandro FELIZ MOK- Univ. Miguel Hernandez (ES)	Synthesis of a perylenediimide-based, triazine-containing non-fullerene acceptor for photovoltaics		
Pres. 4'+1'	Alicia MALDONADO MEDINA-	The Effect of Alkyl Chain Length Interlayer Spacer on the Photobehaviors		
	Univ. Castilla-La Mancha (ES)	of Two New Mn(II)-based Perovskites		
Oral Comm 8'+2'	Mario DE LA HOZ TOMAS- Univ. Castilla La Mancha (ES)	Deciphering the Photochemical Behaviour of a New Tetraphenylethylene Derivative		
	Isabella Antony KALLUVILA JUSTIN- ICMol- Univ. València (ES)	Development of luminescent halide perovskite films through CSS		
	Abhyuday PALIWAL- ICMol- Univ. València (ES)	Efficient vacuum-deposited perovskite solar cells in substrate configuration		
	Daniel HERRERA- ICMAB-CSIC (ES)	From molecules to functionalized devices: design of a lab scale advanced sublimator for direct deposition of organic molecules and its application		
	Rossella ZAFFINO- ICMAB- CSIC (ES)	Integration of curcuminoids into solid-state devices for optoelectronic applications		
	Christian HERNÁNDEZ - Univ. La Laguna (ES)	Multi-functional sensing platform using a luminescent material		
	Lucía MARTÍNEZ GOYENECHE- ICMol- Univ. València (ES)	Narrowband perovskite-perovskite photodetectors using vacuum deposition		
	Arghanoon MOEINI- ICMol- Univ. València (ES)	The effect of fluorinated aliphatic SAMs in vacuum-deposited perovskite solar cells		
	Julia BUJAKOWSKA- Jagiellonian Univ. (PL)	The top-down approach of reducing the {(NH4)[Ni(cyclam)][Fe(CN)6]⋅5H2O}n crystals size		
21h00	Dinner			

	WEDNESDAY 10th			
09h00	Tatjana PARAC-VOGT- KU Leuven (BE)	Metal-oxo clusters and metal organic frameworks as nanozymes		
10h00	Johannes BARTH- TU Munich (DE)	Adatom-mediated chemical conversions and dynamic heterogeneity at surfaces - from catalysis to 2D-materials		
11h00	Coffee break			
11h30	María Antonia HERRERO CHAMORRO- Univ. Castilla-La Mancha (ES)	What can we do with RAMAN in the nanoworld?		
12h00	Reyes CALVO URBINA- Univ. Alicante (ES)	Biaxial compressive strain tuning of neutral and charged excitons in single-layer transition metal dichalcogenides		
12h30	Natxo PASCUAL- CIC NanoGUNE (ES)	Paramagnetism of triangular flakes of graphene		
13h30	Lunch			
15h00	Visit to El Escorial Monastery			
17h30	Fernando MARTIN- IMDEA Nanoscience - UAM (ES)	Attochemistry: Imaging and controlling ultrafast electronic and nuclear motion in molecules at the attosecond time scale		
18h30	Justine HILLAERT- Univ. València (ES)	A robust and predictive platform for the characterization of next-		
	Yousra ASHRAF- Univ. Autónoma Madrid (ES)	Bio synthesis of silver and copper nanoparticles		
	Clara MIRANDA PÉREZ- Univ. Autónoma Madrid (ES)	Characterization of nanoparticle diffusion in a tumor-on-a-chip device		
	Ana ALCOJOR MORENO- Univ. Autónoma Madrid (ES)	Characterization Of Two-Dimensional Perovskites		
	Brecht WEDERHOLDT- ICMol-	Chemically robust metal-organic framework based biocomposites for		
	Univ. Valencia (ES)	their use in biotechnological processes.		
	ICMol- Univ. València (ES)	Engineering Chiral Porosity in Metal-Organic Frameworks		
Flash	Valeria Del Pilar ARIAS	Manufacture and characterization of cellular materials with guest phases		
Pres.	MUNOZ- Univ. Alicante (ES)	for applications in medical implants		
4'+1'	Autónoma Madrid (ES)	Mechanically Interlocked Carbon Nanotubes: Functionalization and Separation of Single-Walled Carbon Nanotubes		
	Clara BOUDEAU- DINANT-	Optical contrast identification of atomically thin-layers of the van der		
	ICMol- Univ. València (ES)	Waals ferromagnet Fe3GeTe2.		
	Estibaliz GIGIREY OLIVA- Univ. Autónoma Madrid (ES)	Preparation of long modified DNA with tunable properties.		
	Víctor CARRATALÁ MUÑOZ-	Programming Amino Acids for controlling Framework Elevibility		
	ICMol- Univ. València (ES) Bafael MOBALES- Univ			
	Autónoma Madrid (ES)	Synthesis of nanoparticles for cell culture and microscopy studies		
	Terriss Mbachick TEKOH - ICMol- Univ. València (ES)	Toward the control of the membrane insertion of a pH-sensitive peptide with light		
	Andrea LÁZARO GÓMEZ-	Development of a second generation of extended triphenylamine-based		
Oral Comm 8'+2'	Ali SHERAZ-ICMol-Univ	High election and strength of ultra-thin metallic transition metal		
	València (ES)	dichalcogenides		
		Localized Strain by Spin Croppover in Ven der Weele Heterectrust		
	Francisco MARQUES MORUS-	Localized Strain by Spin Crossover in Van der Waals Heterostructure		
	ICMol- Univ. València (ES)	Localized Strain by Spin Crossover in Van der Waals Heterostructure		
	ICMol- Univ. València (ES) Elena BRIÑAS GUTIÉRREZ- Univ. Castilla-La Mancha (ES)	Localized Strain by Spin Crossover in Van der Waals Heterostructure Quantification of ultra-trace graphene oxide in real water samples by SERS		

08h00	THURSDAY 11th		
09h00	Guillem AROMÍ- Univ. Barcelona (ES)	Heterometallic Lanthanide Coplexes for Quantum Technologies	
10h00	Fernando LUIS- Univ. Zaragoza (ES)	Wiring up molecular spins with superconducting circuits	
11h00	Coffee break		
11h30	Luis ESCALERA MORENO- MPI für Quantenoptik (DE)	QBithm: towards the coherent control of robust spin qubits in quantum algorithms	
12h15	Matteo BRIGANTI- Univ. Firenze (IT)	Molecular Magnets on Surface: a Dantesque Journey Through the Ab Initio Realm	
13h30	Lunch		
16h30	Sebastian LOTH- Univ. Stuttgart (DE)	Atomic resolution characterization of molecular quantum spins with scanning probe microscopy	
17h30	Andrés MARTÍNEZ GARCÍA- Univ. Alacant (ES)	A user-friendly DFT computational tool to get insight into quantum and spin transport in molecular junctions	
Flash Pres. 4'+1'	María MARTÍ CARRASCOSA- Univ. València (ES)	Synthesis and characterization of the optical properties of SCO nanomaterials in the IR for their integration into nanophotonic devices.	
	Rubén SEBASTIÀ TORRILLAS- ICMol- Univ. València (ES)	Theoretical study of Spin Transition Complexes and their application in Molecular Spintronics	
18h00	Coffee break		
18h30	Klaudia PŁONKA- Jagiellonian Univ. (PL)	Breathing spin crossover coordination framework with elastic frustration controlled by guest molecule adsorption	
Oral Comm 8'+2'	Francisco SÁNCHEZ MARTÍNEZ- Univ. Castilla-La Mancha (ES)	Caged Proton-Transfer Dyes within MOFs for Luminescence Sensing of Acid and base Vapors	
	Dorye L. ESTERAS- ICMol- Univ. València (ES)	Magnon straintronics in 2D materials	
	Maria BRZOZOWSKA- Jagiellonian Univ. (PL)	Molecular intermetallics with unsupported 4f-3d metal-metal bonds as candidates for high-temperature SMMs	
	Shima GHASEMI- Chalmers Univ. Technology (SE)	NBD/QC single molecule electronic switches, effect of chemical anchor groups	
	Aleksander HOFFMAN- Jagiellonian Univ. (PL)	Polar Mn(II)-based multifunctional molecular material exhibiting humidity-sensitive luminescent, magnetic, and electrical properties	
	Jan RZEPIELA- Jagiellonian Univ. (PL)	SHG-active luminescent thermometers from chiral dicyanidoiridates(III)	
	Raul LOPEZ- MARTIN- Univ. Castilla-La Mancha (ES)	Tuning interparticle interactions in closely packed iron oxide nanoparticle assemblies	
20h00	Closing		
21h00	Cocktail dinner	Venue: Hotel Exe Victoria Palace	

#### Flash Presentations & Oral Communications Abstracts

by alphabetical order

ID	SURNAME, Name	ID	SURNAME, Name
08_01	ABELLAN DUMONT, Gonzalo	08_05	MACHÍ HERNÁNDEZ, Jonathan
10_04	ALCOJOR MORENO, Ana	09_09	MALDONADO MEDINA, Alicia
10_07	ARIAS MUÑOZ, Valeria Del Pilar	10_16	MARQUES MOROS, Francisco
08_10	ARTEAGA VINZA, Mercy Elena	11_02	MARTÍ CARRASCOSA, María
10_02	ASHRAF, Yousra	11_01	MARTÍNEZ GARCÍA, Andrés
10_09	BOUDEAU- DINANT, Clara	09_16	MARTÍNEZ GOYENECHE, Lucía
10_17	BRIÑAS GUTIÉRREZ, Elena	08_08	MATEO NAVARRO, Irene
11_07	BRZOZOWSKA, Maria	09_06	MEDINA, Garoé
09_18	BUJAKOWSKA, Julia	10_03	MIRANDA PÉREZ, Clara
10_11	CARRATALÁ MUÑOZ, Víctor	09_17	MOEINI, Arghanoon
09_10	DE LA HOZ TOMÁS, Mario	08_07	MONDÉJAR LÓPEZ, María
09_04	DÉNIZ CORREA, Fernando	08_02	MONTERO, Javier
11_06	ESTERAS, Dorye L.	10_12	MORALES, Rafael
09_03	FARRANDO PÉREZ, Alex	08_14	MORCILLO MORA, Alicia
09_08	FELIZ MOK, Jose Alejandro	08_06	NASIRI , Mohammad Ali
09_05	FERNÁNDEZ DE LA FUENTE, Mario	08_11	NIZA GONZÁLEZ, Enrique
11_08	GHASEMI, Shima	09_12	PALIWAL, Abhyuday
10_10	GIGIREY OLIVA, Estibaliz	11_04	PŁONKA, Klaudia
09_01	GOMAR FERNÁNDEZ, Mª Inmaculada	08_12	PRADO SOCORRO, Carlos David
10_06	GÓMEZ TENÉS, Guillermo	09_02	ROYO DE LARIOS, Álvaro
09_15	HERNÁNDEZ ÁLVAREZ, Christian	11_10	RZEPIELA, Jan
09_13	HERRERA, Daniel	08_13	SALHI, Juba
10_01	HILLAERT, Justine	11_05	SÁNCHEZ MARTÍNEZ, Francisco
11_09	HOFFMAN, Aleksander	11_03	SEBASTIÀ TORRILLAS, Rubén
08_03	HURTADO, Violeta	10_15	SHERAZ, Ali
10_08	JIMÉNEZ MERINO, David	10_13	TEKOH, Terriss Mbachick
09_11	KALLUVILA JUSTIN, Isabella Antony	10_05	WEDERHOLDT, Brecht
10_14	LÁZARO GÓMEZ, Andrea	09_07	XIMENIS CAMPINS, Pedro
08_90	LIZALDE ARROYO, Félix	09_14	ZAFFINO, Rossella
11_11	LOPEZ- MARTIN, Raul	08_04	ZAMORA AMO, Esteban

#### Chemical Transformations in COFs Driven by Light and pH Stimuli

Raquel Gavara Castell,<sup>1</sup> Gonzalo Abellán Dumont,<sup>1</sup> Félix Zamora.<sup>1,2</sup>

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The development of two-dimensional nanomaterials has gained significant attention in the field of new materials research due to their great technological potential. COFs (Covalent Organic Frameworks) are especially on the rise. Due to their structure, bidimensional COFs have various applications such as gas separation by adsorption. In this field, there is a great interest on the preparation of COF nanosheets or CONs, which exhibit a nanometric thickness, making them suitable for new applications.[1] These nanosheets can be prepared by means of a top-down approach, through the exfoliation of the material. In this work, **[HC=C]**0.5-**TPB-DMTP-COF** and **[HC=C]**0.17-**TPB-DMTP-COF** have been synthesised and then functionalised with the photoactive species of a flavylium type molecule, the *trans*-chalcone **Ct**, to form **Ct**0.33-**COF** and **Ct**0.17-**COF** (Figure 1), respectively. **Ct** undergoes a sequence of chemical transformations when is irradiated with UV light or when is heated, at the appropriate pH range, giving rise, to a positive-charged species, the flavylium cation **(AH+)** (Figure 1).[2] The formation of this species could provoke the exfoliation of the COFs, due to electrostatic repulsions between their bidimensional layers.

Thus, aqueous dispersions of the functionalized COFs at different pH values, have been subjected to either UV irradiation or heat to study the conversion from **Ct** to **AH+** within the **Ct-COF** and analyse the different physic-chemical properties that the **COFs** functionalized with each of the flavylium species (**Ct** or **AH**<sup>+</sup>) exhibit. Besides, we will try to exploit the photochemical response of **Ct** for the controlled release and capture of other molecules.



Figure 1. Overall equilibrium between Ct and AH+ species. Ct<sub>0.17</sub>-COF

#### <u>References</u>

Chalcona trans (Ct)

- [1] Rodríguez-San-Miguel, D.; Montoro, C.; Zamora, F. Covalent Organic Framework Nanosheets: Preparation, Properties and Applications. *Chem. Soc. Rev.* 2020, 49 (8), 2291–2302. https://doi.org/10.1039/C9CS00890J.
- [2] Pina, F.; Melo, M. J.; Maestri, M.; Ballardini, R.; Balzani, V. Photochromism of 4'-Methoxyflavylium Perchlorate. A "Write-Lock-Read-Unlock-Erase" Molecular Switching System. J. Am. Chem. Soc. 1997, 119 (24), 5556–5561. https://doi.org/10.1021/ja9704646.

### Efficient and selective thiosemicarbazones for heavy metal sequestration from water. Aqueous Stability studies of their stable nontoxic materials

Javier Montero Gutiérrez<sup>1</sup>, Carmen Viciana<sup>1</sup>, David Fabra Ana Matesanz<sup>2</sup>, Adoración G. Quiroga<sup>3</sup>, Edouardos Loukopoulos<sup>4</sup>, Ana Platero<sup>5</sup>, Isabel Sanchez<sup>6</sup>.

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Among all the contaminants that can affect the water viability, heavy metals can produce alarming effects due to their slow chemical and physical degradation over the time [1]. Thiosemicarbazones are versatile heavy metal chelators, and we consider them a good choice as compounds to remove metallic ions from an aquatic environment [2]. The compounds formed with the metal ions can be additionally immobilised in solid structures such as metal organic frameworks (MOFs). These platforms allow heterogenous separation of metals from water. MOFs are promising materials for this task because of their large adsorption capacity and tunable pore size and structure designIn this study we are using MOFs in collaboration with Ana Platero's group, because their MOF's library has shown a remarkable stability in aqueous solutions [3]. This library contains promising candidates and some of them are built from unsaturated Zr6O8 clusters linked by carboxylate derivatives. The MOF can be activated and can serve as a scaffold to insert discrete functional groups [4]. Our initials attempt of MOF-functionalization was performed just with the TSCN in solution, but the process was not as efficient as expected. The studies of the TSCN'S chemical stability showed that some of them were not stable in an acidic aqueous solution due to a hydrolyzation process. However, the coordination of heavy metal such as Ni inferred an extra stability that allows the mechanical functionalisation. Our aim is to achieve a nontoxic platform to remove heavy metal ions using TSCN and TSCN immobilized with MOFs. We will evaluate the stability in water of the final compounds, their toxicity in cells and the possible interactions with biological models.

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In this work the fabrication of nanocomposite polycaprolactone-based electrospun nanofibers designed for nitrates removal from water is presented. Nitrates are progressively more present in nature and open waters due to human activity, and they are potentially toxic for human health [1]. To face this problem, there is a list of available nitrate-cleaner technologies from water, but their technological complexity doesn't allow to apply them directly on the polluted environment, which reduces drastically their applicability. To solve this limitation, a novel approximation has been proposed: the design and production of nanocomposite materials using modified sepiolie, which could adsorb contaminants directly from polluted water. In this way, a big step has been done with the production of nanocomposite hydrophilic polyurethane foams, which act as a sustainable matrix where the active principle for this process, treated sepiolite, is dispersed [2]. This approach allows the stable encapsulation of nanoparticles, which cannot migrate into the environment, and moreover, open the door for the potential reusability of the new material. However, nitrates removal times rise following this approach, requiring of further optimization for its successful implementation on continuous processes.

Herein, the encapsulation of quaternary ammonium salts modified sepiolites in electrospun nanofibers is proposed in this work to enhance the kinetics and the performance of the adsorption process. This type of fibrous materials are well known to have a high surface area to volume ratio, while maintaining very good mechanical properties [3], becoming a high-performance material for this application.

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#### Exfoliation of non-laminar materials

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Liquid phase exfoliation (LPE) of laminar structures has been done for more than ten years, creating suspensions of 2D materials by breaking weak interlayer van de Waals interactions. Thus, it was believed that LPE was not possible in non-laminar structures. It has been in the recent years that exfoliation of this kind of materials has been proven that can be made by the breaking chemical bonds of the structure. <sup>[1]</sup> The optimization of the processes needs to keep improving to take advantage of these new materials and their properties. The research on these types of materials can open the possibility of new applications in optics, electronics, or catalysis. <sup>[2] [3]</sup>

We are studying the optimization of the LPE in non-layered materials such as pyrite and hematite, by applying different procedures such as wet ball milling, tip sonication and ultrasound bath, changing different parameters to increase the size of the nanosheets produced. In this work we will show the resulting nanolayers by atomic force microscopy, scanning electron microscopy, transmission electron microscopy and Raman spectroscopy.



Figure 1: We observe the process of exfoliation of pyrite starting from the ore material a) and through a process of agate mortar and wet ball milling we obtain our base powder b) which is then sonicated in isopropanol to obtain our suspension of nanosheets c), and afterward the sheet morphology is analyzed d).

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#### Heterometallic ZIF-8 analogues for light hydrocarbon separation

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The development of porous materials for gas sorption has become an important topic in material science due to its importance in purification, gas storage, and separation processes [1]. Among these materials, metal-organic frameworks (MOFs) have emerged as one of the most promising alternative due to their tunability and large surface areas, allowing efficient selective gas separations in chemical engineering industry [2].

In particular, methane extraction from natural gas is one of the main challenges of the current global energy market [3]. For this reason, novel materials must be capable of separating light hydrocarbons traces from methane streams. This research is pointing to the future implementation of metal-organic frameworks in gas industry.

ZIF-8(Zn) is one of the most reported MOFs and its adsorption properties have been widely studied. Now, using a previously reported solvent-free approach [4], and aiming to improve the selectivity towards  $C_2$ ,  $C_3$  and  $C_4$  hydrocarbons, we synthesized a set of Fe:Zn heterometallic analogues of ZIF-8. Moreover, we water-degraded those materials to favour the creation of mesopores; without kinetic impediments, methane purification can be now thermodynamically driven. Industrial gas separation performance will be studied using a gas breakthrough setup.



Figure 1.- SEM images of ZIF-8 analogue (90:10-Fe:Zn). a) before degradation; and, b) after degradation.

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### Optimization of thermoelectric polymer-based generator embedded into a meta-surface absorber

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In this work, the performance of a thermoelectric generator module was enhanced by embedding a thermoelectric polymer cell into a meta-surface absorber to optimize sunlight absorption [1]. The optical and thermoelectric properties of the resulting device are optimized separately and combined in a single device. The optical components consist of a transparent substrate, a high refractive index material, low refractive index (RF) material and finally a semi-transparent metal. The complete device is made of a sapphire substrate, covered with a thin silicon layer, a transparent thermoelectric copolymer and an ultrathin nickel film [2-3]. This way, we can add contacts on the copolymer to fabricate the thermoelectric device. First, the Transfer-Matrix Method (TMM) was used to parametrize the absorption of the resulting device in terms of the thickness of the different layers considered. The results point to an optimal absorption for the case of silicon thin films with 112 nm of silicon, 429 nm of PEDOT:PSS BTFMSI, and 6 nm of nickel. Importantly, the numerical results showed that the systems exhibited certain robustness related to the layer thicknesses. Secondly, two electrochemical techniques, including pulsed and chronoamperometry approaches, were used to obtain an optimal PEDOT:PSS BTFMSI layer. During the optimization, AFM analysis revealed that films created using the electrochemical pulsed method have low roughness (less than 10 nm RMS). After checking the performance of the multilayer structure, the transparent nickel film was patterned by micro-lithography increasing the Seebeck coefficient and hence performance of the thermoelectric module. Figure 1 shows Schematic of the optimal structure to maximize the absorption energy in the broadband wavelength.



Figure 1. Schematic of the optimal structure to maximize the absorption energy in the broadband wavelength.

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#### Polysaccharide film containing chitosan nanoparticles for food preservation

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Nanotechnology techniques are also used to encapsulate essential oils to improve their stability, pharmacological properties and physicochemical properties. Specifically, essential oils encapsulated in biopolymeric nanocarriers reveal favorable antimicrobial and antioxidant activity, being suitable materials for active food packaging thanks to the inhibition of microbial growth in different food products [1]. Due to the previously mentioned, this study was developed to evaluate the activity of a film containing nanoparticles for active food packaging. Transcinnamaldehyde was encapsulated in chitosan nanoparticles and this synthesis was carried out by the ionic gelation method. Nanoparticles were obtained with a radius size of 89.80 nm, PDI of 0.41 and Z potential of 27.40 mV. Regarding film properties, a thickness of 0.122 mm and an elongation at break of 76.50% were obtained. The result of the release process was a first stage characterized by a faster release during the first 5h reaching 47% of transcinnamaldehyde, followed by a slower and more progressive phase that achieves 100% of transcinnamaldehyde during the following 96 h. Consequently, the preservation properties of the film indicated a stronger initial protection against possible bacteria, followed by a more sustained release period in which cinnamaldehyde is still being released to preserve the shelf life of the product. In addition, a significant reduction in total aerobic bacteria and total coliforms was observed during 10 days of storage. Finally, a challenge test with L. Monocytogenes was performed to quantify the bacteria according to the conditions defined to be expected between production and consumption.

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### Synthesis and photophysical study of an azobenzene-containing oblique perylenediimide dyad

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Naturally occurring photosynthesis is a chemical process that involves the conversion of inorganic matter into organic matter thanks to the energy of sunlight. One of the key steps in this process is based on a phenomenon called photoinduced electron transfer (PET), which is the transfer of an electron from a previously excited donor molecule to another acceptor one. PET has been extensively studied for its application not only in artificial photosynthesis, but also in optoelectronics and photovoltaics [1].

Perylenediimides (PDIs) are an important family of dyes with high thermal and chemical stabilities, whose chemical functionalization allows the modification to a great extent of the optic and electronic properties of the compounds. As a consequence, they have been extensively studied in PET processes [2].

Recently, we have prepared and characterized a couple of dyads formed by two PDIs linked by azobenzene bridges through their bay positions. Depending on the nature of the atom bridging the PDI core and the azobenzene, we were able to detect either quadrupolar ultrafast charge transfer (N as the linking atom) or symmetry-breaking charge separation (O as the linking atom) [3].

In this presentation, we will introduce a new dyad combining O and N atoms as bridging motifs between the azobencene and the PDIs, together with an oblique arrangement of the PDIs.



Dyad 1

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### The future of cellular materials: High-Performance and Transparent Nanocellular Polymers

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In recent years, the development of high-performance polymers has revolutionized the field of materials science. These polymers have superior mechanical, thermal, and chemical properties compared to conventional polymers, making them highly sought after in a variety of industries [1]. On the other hand, nanocellular polymers, cellular polymers with cell sizes in the nanometric scale, have emerged as a promising approach to producing lightweight, low thermal conductivity and transparent materials with good mechanical properties [2,3].

The combination of the benefits of high-performance polymers and nanocellular polymers opens up new possibilities for developing materials with improved properties while maintaining their existing mechanical performance.

By incorporating nanocellular structures into high-performance polymers, it is possible to achieve materials with a reduced weight, low thermal conductivity, among other properties, while maintaining the transparent character and the mechanical performance. If the cell size is small enough it is expected that this material could have even greater strength or toughness than the performer solid polymer. Materials resulting from this combination hold great promise for applications in sectors such as construction and automotive, where lightweight and high-strength materials, as well as increased energy efficiency, are desired.

In this work, we report for the first time the generation of transparent high-performance nanocellular polymers. In particular, nanocellular polymers based on polyetherimide (PEI) were produced. The effect of the processing conditions on the density, structure and properties of the materials is evaluated. Results prove that a specific design of the processing parameters is needed to achieve structures with the desired characteristics and properties.

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#### Amphiphilic Scorpiand-like Complexes as Superoxide Dismutase Mimics.

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Living organisms rely on Superoxide Dismutase (SOD) enzymes to protect themselves from the deleterious effects of the superoxide radical. SODs are a family of enzymes that remove highly reactive superoxide radical anions  $(O_2^-)$  and catalyze their dismutation into the non-radical species dioxygen and hydrogen peroxide.<sup>1</sup> In humans, alterations in these protective mechanisms have been related to the pathogenesis of many diseases. However, the therapeutic use of the native enzyme is hampered by, among other things, its high molecular size, low stability, and immunogenicity.2,3



*Figure 1*: *MnSOD* mechanism and crystal structutre of a synthetic mimic for this enzyme.

In this communication, we present the synthesis, properties, and SOD-like activity for some **scorpiand-like ligands** with **amphiphilic properties**. These ligands form stable pentadentate complexes with electroactive metals such as Cu(II) and Mn(II) as the metal core. Their macrocyclic core is similar to the active center of native MnSOD. Its SOD-like activity has been tested by the McCord-Fridovich test and all of them are capable of SOD-like activity. Hydrophobic pending groups of different lengths modulate the overall hydrophobicity and seem to have an important role in the membrane permeability. The introduction of N-methyl groups also increases the permeability.

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#### Chitosan coated - biogenic silver nanoparticles from wheat residues as green antifungal and nanoprimig in wheat seeds

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In this study, chitosan-coated biogenic silver nanoparticles (AgNP-CH) were obtained through green chemistry by recycling wheat crop leaf residues. The nanoparticles were characterized by UV-VIS spectroscopy, and total reflectance-Fourier transform infrared spectroscopy confirmed the nanoparticle formation, and the incorporation of chitosan surrounding silver nanoparticles. The size and morphology of nanoparticles were evaluated by microscopy techniques, showing a size range of 2-10 nm, with spherical shape and narrow distribution. The antifungal assay indicated a higher antimicrobial activity showing values of minimum inhibitory concentrations of 41.7 µg/mL against Fusarium 208.37 µg/mL oxysporum, and for Aspergillus niger, A. versicolor and A. brasiliensis. Finally, non-phytotoxic effects were observed in germination assays at early plant stage of development, and an increase in chlorophyll levels were observed at the doses tested with AgNP-CH. Thus, the use of AgNP-CH could be a potential alternative for the prevention of fungal infections in cereals in the early stages of wheat crop development [1].



Fig.1 Chitosan-coated silver nanoparticles obtained through a circular economy approach

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#### Quantifying the Effects of Varying Polymer Electrolyte Concentrations on the Memristive Properties and Circuit Models of Organic Devices

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Memristive materials hold great potential for neuromorphic technology as they integrate information processing and memory storage in a single component. In this study, we investigate the memristive properties of a two-terminal organic device based on ionic migration facilitated by an ion-transport polymer [1]. Specifically, we explore the effects of varying mass ratios between the ion-conductive polymer, ion-containing salt, and semiconductive polymer on the device's memristive properties. Using impedance spectroscopy, we measure the intrinsic ion mobility in the devices and design equivalent circuit models to characterize their capacitive, resistive, and inductive behavior. Our work sheds light on the impact of chemical interactions between ions and their ion-conductive mediators on the memristive properties of these devices. We also discuss the transport mechanism under an AC field, providing a deeper understanding of their dynamic behavior. Our findings contribute to the development and optimization of organic memristive devices for future applications in neuromorphic computing.



Figure 1. 16-pin organic memristive device based on a mixture of polymers sandwiched between the ITO and Ag electrodes.

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#### New strategy towards periodically organized polyoxometalates on HOPG for molecular electronics applications

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Polyoxometalates (POMs) are widely studied for the development of new materials for molecular electronics<sup>[1-3]</sup>. Indeed, they present several interesting redox and magnetic properties <sup>[4]</sup>. Nevertheless, despite several attempts<sup>[5]</sup>, one key limitation is the difficulty (or impossibility in soft conditions) to organize POMs periodically at a molecular scale on a surface, isolated from each other and isolated from the substrate as well, to allow them to be addressed individually. Indeed, POMs are charged species and tend to form aggregates due to POM-POM electrostatic interactions.



In order to sort out this challenge, here we present a relatively simple approach using a molecular template<sup>[6]</sup> made of an HOPG surface-confined self-assembly of triazine-based molecules. The protonation of the self-organized triazine layer in presence of an heteropolyacid allowed the non-covalent anchoring of the POMs on specific sites of the surface by electrostatic interaction. The system was characterized at different scales, from macroscopic to molecular level using various techniques. In particular, after presenting our chemical strategy, X-ray Photoemission spectroscopy (XPS), Field Electron Gun - Scanning Electron Microscopy (SEM-FEG) with X-ray Energy Dispersive spectroscopy (EDX) as well as near-field microscopies were carried on to evidence respectively the presence of the ammonium signal, and/or of the POMs on the surface, as well to image the surface at the nanometric and molecular scales.

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#### Synthesis and characterization of self-healing materials.

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Soft materials such as polymers, elastomers or hydrogels can be easily damaged, for that reason, their lifetime, in most cases, is too short. This problem has led, in the last years, to the study of self-healing materials. Different self-heling mechanisms have been studied and the most important are: i) encapsulation of selfhealing agents, ii) metal-ligand coordination bonds, iii) reversible covalent bonds such as Diels-Alder reactions, iv) non-covalent bonds such as hydrogen bonds or ionic interactions or hydrophobic interactions [1]. Some of the previous mechanisms are not autonomous, which means that the material must receive an external stimulus like light, heat or a magnetic or electric field to have self-healing, for that reason these materials do not have many applications. The objective of this work is to find hydrogels with autonomous self-healing and with good mechanical proprieties. The starting point is the SHAP hydrogel (Self-Healing AETA-based Polymer) [2], this hydrogel was synthesized by photopolymerization of (2-(Acryloyloxy)ethyl)trimethylammonium chloride (AETA) using N,N'-Methylenebisacrylamide (MBA) as the chemical crosslinker and sodium 2,4,6-trimethylbenzoylphosphonate (NaTPO) as photoinitiator in water. The self-healing capacity of this hydrogel is given by the hydrogen bonds that form the water molecules inside the structure. To improve this capacity, monomers with diverse charges were added to the SHAP chemical structure producing an additional electrostatic interaction between the different monomers. Different hydrogels were synthesized using various types of negatives and positives monomers and different molar concentrations.

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#### **Close-Space Sublimation for Development of Efficient Perovskite Solar Cells**

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Organic–inorganic hybrid perovskite solar cells have gained popularity in the past few years for photovoltaics. This is possible because of their suitable characteristics such as tolerance to defects, tuneable bandgap and high absorption coefficients. Perovskites are a crystallographic family with a general ABX<sub>3</sub> structure (being A=monovalent cation; B= divalent cation and X= monovalent anion). In this work, close-space sublimation was used to convert inorganic thin films into perovskite films and then made into solar cells. The composition was  $Cs_{0.1}FA_{0.9}Pb(I_{0.9}CI_{0.1})_3$ . Finished devices were characterized with x-ray diffraction, showing that we do not get any yellow phase. We performed stability tests by annealing samples for long periods of time (>month) to study how their efficiency, open circuit voltage and short circuit density vary over time. The most efficient device was achieved by using TaTm doped with CS-9 as a hole transport material and C60/SnO<sub>x</sub> as electron transport layers. In this work, a maximum efficiency of 18.7% was achieved with a short circuit density 24 mA/cm<sup>2</sup> and open circuit voltage of 1.03V after four weeks at 85°C in a nitrogen atmosphere.

### Computational study of hydrogen-bonded organic frameworks based on tetrathiafulvalene building block and its selenium/tellurium analogues.

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Tetrathiafulvalene (TTF) structures are known as good electronic donors and can be used as a building block to form electroactive 3D materials. <sup>[1]</sup> Recently, this unit has been exploited in hydrogen-bonded organic frameworks to engender semiconductivity in porous materials (MUV-20a and MUV-20b). <sup>[2]</sup> The efficient charge transport in these systems was described by the presence of a zwitterionic species promoted by spontaneous oxidation of the TTF moiety, which assembles in a  $\pi$ - $\pi$  stacking with a through-space charge-transfer from one TTF to its neighbors.

In order to enhance the conducting properties of this family of HOFs, a theoretical and computational study has been performed to analyze the impact of replacing the sulfur heteroatoms of TTF with other chalcogenide elements such as selenium and tellurium, or having a mixed chalcogenide system (e.g. triselenathiafulvalene - TSTF). <sup>[3]</sup> First, the isolated ligand derivatives are analyzed based on molecular calculations at the DFT-B3LYP level of theory using the Gaussian-16 program suite. Then, we compute the minimum-energy crystal and electronic structure of the different materials in periodic conditions using the FHI-AIMS software, and obtain the characteristic charge transport parameters for this family of chalcogenide HOFs.

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#### Near-Infrared Lasing in Perylene-Based Linear Non-Alternant Nanoribbons.

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The study of nanographenes (NGs) as near-infrared (NIR) emitting compounds have awakened great interest due to its potential integration in telecommunications and biomedical applications [1] [2]. Here, the optical and amplified spontaneous emission (ASE) properties of three linear non-alternant nanoribbons (NNRs) dispersed in polystyrene films are investigated. These NNRs feature pentagonal rings and their size is increased by repeating a unit of perylene [3]. Results show that the annulated pentagons play an important role regarding the optical properties. The NNRs exhibit strong photoluminescence (PL) and ASE thresholds significantly lower than those of other NIR-emitting NGs [4]. The increase in the number of perylene units in the compound results in a red-shift of the PL emission (PL at 741 nm in the larger compound). Besides, the photostability of the larger NNRs is outstanding: under pumping at very extreme conditions at the same spot of the sample, the ASE intensity keeps nearly the same after more than 10<sup>5</sup> pump pulses (10 Hz, 4.5 ns). The potential of the materials for red and NIR lasing is demonstrated through the fabrication of distributed feedback lasers with top-layer resonators.

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#### New optical active doped perovskites based on ytterbium.

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Nowadays, there is a great deal of interest in the exploration of the structure, particle-size, and active-ion-concentration dependent luminescence properties of trivalent lanthanide (Ln<sup>3+</sup>)-doped perovskites for a wide range of applications [1], such as solar cells, LEDs, IR detectors and IR-Visible converters; directly related to one of the most outstanding properties, up-conversion.

A complete control of the photophysical (structure vs luminescence) properties of these systems is highly necessary for their design and development [2], so that's why Yb<sup>3+</sup>, Yb<sup>3+</sup>/Tl<sup>3+</sup>, Yb<sup>3+</sup>/Er<sup>3+</sup> co-doped in different concentration SrMoO<sub>3</sub> perovskites were synthesized by ceramic method and characterized by DRX and SEM showing the real structure.

Moreover, the perovskites were studied theoretically, focusing on dopants, for future optical study. In this way it has been possible to visualise the emission, absorption, excitation and lifetime spectra of the lanthanides, as well as one of the most important factors in this study, the up-conversion.



Figure 1: Emission spectra of Yb/Er doped perovskite

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#### **Open-Cell Nanocellular Polymers:**

#### A Promising Solution for Green Insulation and Filtration.

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The study of cellular polymeric materials [1] (biphasic materials in which a gas is dispersed in a solid polymeric phase), has been of great interest during the last decades. The same way, development of materials that can help mitigate environmental problems has become a crucial necessity [2]. In recent years, nanocellular polymers have emerged as a promising solution in this search.

These materials have cellular structures with nanometer-sized pores that give them unique properties such as low thermal insulation, high surface-to-volume ratio, weight reduction, and transparency. These properties make them have a great presence in technological sectors such as construction, packaging, the automotive industry, etc. That is why by controlling the manufacturing process, materials can be obtained "à la carte", a very important aspect for the industry.

Their potential applications are vast, but many of them can only be realized if the pores are interconnected, creating an open-cell structure. Open-cell nanocellular materials hold great potential for two critical applications: insulation and filtration. In the insulation sector, reducing emissions and energy consumption due to heating and cooling is a major challenge. One solution is to use Vacuum Insulation Panels (VIP) that require open-cell materials inside to create a vacuum. However, current solutions are expensive and not environmentally friendly. Similarly, in the filtration industry, the demand for smaller and smaller cells to filter out harmful particles is growing.

To address these challenges, this study proposes the fabrication of open-cell nanocellular foams from PMMA gels using a simple and environmentally friendly process [3]. Starting from a gel allows for the easy production of open-cell structures, resulting in a 90% reduction in cycle time and energy consumption [4]. The use of nanotechnology in this study provides a significant opportunity for the development of sustainable and efficient materials with a broad range of applications.

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### Structural and Optical Characterization of new lanthanide doped perovskite type oxides.

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Abstract body: The synthesis of the perovskite-type oxides with formula  $A'_xSr_{1-x}MoO_3$  (A'= Er, Nd) by the ceramic method has been carried out and, subsequently, the structural characterization by means of X-ray diffraction and scanning electron microscopy has been done; based on this analysis both symmetry and punctual group of the perovskite have been verified. The optical characterization has been carried out by using laser spectroscopy [1]. It consisted on the emission and excitation spectra in the Vis-IR range, lifetime of relevant excited states and therefore the study of the relationship between the dopant concentration and the relaxation phenomena [2] as shown in figure 1, and to sum up, the upconversion intensity.



Figure 1. Lifetime of excited states of Er<sup>3+</sup> at different concentrations

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#### Synthesis and self-assembly studies of $\pi$ -conjugated dipyrrolidones

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Precise and controlled self-assembly of  $\pi$ -conjugated small organic compounds (or dyes) is crucial to develop optoelectronic materials with suitable molecular organization to enable the optimal charge transfer between the overlapping orbitals.[1] Such control can be achieved by careful molecular design of the monomeric building blocks. One of the strategies to obtain well-ordered dye structures is to incorporate in the  $\pi$ -conjugated scaffolds hydrogen bonding units that guide the assembly process into well-defined and robust supramolecular nanostructures.[2] For example, aromatic pyrrolidones are small dyes that fuses a five-membered lactam ring (pyrrolidone) with aromatic scaffolds. This configuration provides the ability to the molecules to interact via hydrogen bonds between the amide NH and the C=O groups, but also a high conjugation. As a result of that, aromatic pyrrolidones are of interest for self-assembly studies, but are also good candidates to develop supramolecular materials with good semiconducting properties.[3]

Herein, we have designed two novel  $\pi$ -conjugated dipyrrolidones: benzodipyrrolidone (BDP) and naphthodipyrrolidone (NDP) (Figure 1). Both compounds are functionalized with two wedge-shaped groups, which may provide solubility in organic solvents and liquid-crystalline properties. The new compounds are expected to self-assemble via complementary hydrogen bonds (figure 1) and  $\pi$ - $\pi$  interactions, forming one dimensional assemblies in solution and/or in bulk.



Figure 1. Structure and expected self-assembly mode of the newly prepared π-conjugated dipyrrolidones: a) BDP, b) NDP.

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### Synthesis of a perylenediimide-based, triazine-containing non-fullerene acceptor for photovoltaics

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Perylenediimides (PDIs) display a high chemical versatility that allows applicationoriented tailoring of their optical and electronic properties [1]. This, together with their high stability against heat, radiation and chemicals, led to their application in a wide variety of fields, as for example in photovoltaics [2].

In this presentation, we will describe the synthesis and characterization of a novel non-fullerene acceptor molecule bearing four PDI units linked to electron-poor triazine rings. The goal is to gain valuable insights into the design of efficient and cost-effective materials for renewable energy applications.



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#### The Effect of Alkyl Chain Length Interlayer Spacer on the Photobehaviors of Two New Mn(II)-based Perovskites

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Mn(II)-based perovskites have been researched extensively due their promising nonlinear optical properties and tunable luminescence arising from the different coordination environment of Mn<sup>2+</sup> due to the <sup>4</sup>T<sub>1</sub>-<sup>6</sup>A<sub>1</sub> transition.[1,2] In adittion, this type of perovskites could replace the toxic Pb<sup>2+</sup> although there are still some obstacles to get over, like stability, sensitivity to humidity, color tunability, etc. [3] In this work, we will show our recent results for two Mn (II) bromide perovskites exploring the effect of monovalent (P1) and bivalent (P2) alkyl interlayer spacers (Figure 1A).[4] P1 displays an orange-red emission with a quantum yield of 3.6%, whereas P2 shows a green photoluminescence, with quantum yield of 26%. We explain the result in terms of different Mn<sup>2+</sup> coordination, electron-phonon couplings and Mn-Mn interactions. We demonstrate that the encapsulation of P1 and P2 in PMMA film improves their stability against humidity (Figure 1B). Their emission intensity decreases with no significant spectral change when we increase the temperature due to stronger electron-phonon interactions. The emission decays fit two microsecond components -the shorter one  $(\sim 100 \ \mu s)$  is asigned to hydrated phases and the longer one  $(\sim 300 \ \mu s)$  - to nonhydrated ones (Figure 1C). Our findings provide insights into the effects of linear mono- and bivalent organic interlayer spacers on the photophysics of perovskites.



Figure Structures 1. (A) of C<sub>2</sub>H<sub>5</sub>NH<sub>3</sub>MnBr<sub>3</sub> (P1) and C<sub>2</sub>H<sub>4</sub>(NH<sub>3</sub>)<sub>2</sub>MnBr<sub>4</sub> (P2) perovskites using mono- and bivalent organic spacers, respectively. (B) Change (ambient humidity, 50-60%) in the emission intensity maximum (normalized to 1) with time of neat and PMMA-protected P2. (C) Comparison of the photoluminescence decays of P1/PMMA (red) and P2/PMMA (green) following excitation at 433 nm.

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#### Deciphering the Photochemical Behaviour of a New Tetraphenylethylene Derivative

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Tetraphenylethylene (TPE) derivatives have become one of the most versatile building blocks with aggregation-induced emission (AIE) due to its facile functionalization and use in numerous applications. [1,2] However, its applications are limited by the photophysical and photochemical processes that occur in their excited state. [3] Here, we report a detail study of the photochemical behaviour of a new TPE derivative with terphenyl groups (TTECOOBu) in solvents with different viscosity and in PMMA film. Irradiation experiments under UV light show an efficient photocyclization reaction, which gives a 9,10-diphenylphenanthrene (DPP) derivative. The emission spectra in solutions show that the intermediate species (~ 420 nm) is stable and does not revert to its initial state, and in presence of oxygen it is rapidly photo-oxidized to the final DPP derivative (~ 380 nm) with an enhancement in photoluminescence efficiency (Figure 1). We demonstrate that photocyclization reaction is more efficient in solvents with increasing viscosity or in a rigid matrix (PMMA film), where the torsional motions of phenyl rings are hindered. We also elucidated the femto to millisecond photodynamics of the intermediate and final photoproducts and provide a full picture of their relaxation, being the later one living in ~ 1 ns at  $S_1$  and ~ 1  $\mu$ s at  $T_1$ .



**Figure 1.** A) Molecular structure of **TTECOOBu**. B) Changes in the absorption and emission ( $\lambda_{exc}$  = 325 nm) spectra of **TTECOOBu** in DCM solutions for different periods of irradiation using an UV-light at 365 nm (UV<sub>MAX</sub> = ~ 0.3 W cm<sup>-2</sup>).

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## Development of luminescent halide perovskite films through CSS

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Lead halide perovskites have recently emerged as promising low-cost candidates for many optoelectronic applications, including perovskite light-emitting diodes (PLEDs). Among different compositions, 2D or quasi-2D systems exhibit outstanding optical properties, given their inherent quantum-well structure and large exciton binding energy, which results in high photoluminescence quantum yields (PLQYs). Despite the vast majority of PLEDs rely on solution processed thin films, vacuum deposition is a solvent-free and scalable alternative that could have superior control over film thickness and composition. <sup>[1]</sup> Yet, vacuum deposited low dimensional perovskites are still rare given the instability of ammonium salts under heat and high-vacuum conditions.

Here, we report a 2-step solvent-free deposition method using a low-vacuum close-space sublimation (CSS) tool. Given that the distance between the source and the substrate is very small (<5mm), this technique requires very low vacuum conditions, allowing the use of alternative, instable ammonium salts. Starting from a thermally evaporated precursor film, we investigate state-of-the-art 3D compositions and their PL properties after incorporating several surface passivates. Similarly, luminescent 2D and quasi-2D systems based on benzylammonium-FABr lead bromide have been investigated. Interestingly, we observe fast deposition and a high perovskite conversion rates for most of the systems, which are highly dependent on the sample temperature and chamber pressure. In addition, the quasi 2D system does not evolve into different *n* dimensionalities with the incorporation of FABr, but it rather segregates into two defined systems with independent PL, providing a stable and defined light emission spectra.

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## Efficient vacuum-deposited perovskite solar cells in substrate configuration

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Lead halide perovskite solar cells (PSCs) have rapidly advanced over a short time period, achieving power conversion. efficiencies (PCE) above 25% and enhanced stability for single-junction solar cells. These devices, however, are fabricated in superstrate-configuration over transparent conducting electrodes which are adequate for fabricating small area cells, but not for large area cells that are employed in modules due to resistive losses. This limitation can be overcome by fabricating PSCs in substrate-configuration on highly conductive and reflective metal films. Further, the absence of 'glass' in the path of light upon illumination in this case could be leveraged to minimize optical losses in the device and achieve high current densities.<sup>1</sup> To this end, in this work, we demonstrate efficient, all vacuum processed PSCs in substrate configuration. The resultant devices (~0.05 cm<sup>2</sup>) having a co-evaporated formamidinium methylammonium lead iodide (FAMAPI, Eq of ~1.54 eV) perovskite demonstrate a maximum power conversion efficiency (PCE) of ~19%, which is comparable to the maximum PCE of ~19.5 % obtained in the superstrate configuration devices and is the highest value reported for a PSC in substrate configuration. The devices in substrate configuration exhibit higher short circuit current density values despite the parasitic absorbance from the front fullerene- $C_{60}$  layer (> 0.5 mA/cm<sup>2</sup>). Next, we observe that the encapsulated devices of both the configurations exhibit similar thermal stability at 85 °C (on hotplate) in N<sub>2</sub> environment, reaching a  $t_{80}$  (time to reach 80% of the original PCE) of ~800 hours.



Figure: Picture of small area vacuum deposited perovskite solar cells in substrate configuration.

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## FROM MOLECULES TO FUNCTIONALIZED DEVICES: DESIGN OF A LAB SCALE ADVANCED SUBLIMATOR FOR DIRECT DEPOSITION OF ORGANIC MOLECULES AND ITS APPLICATION

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In organic molecular electronics, a growing area in the recent years, the rapid screening and testing of potential molecules is critical. In this sense, we faced with the problem of how we could deposit new organic molecular candidates onto different devices or solid substrates for their evaluation, but in a green and straightforward manner, minimising the number of steps and for use in a standard chemistry laboratory.

The deposition of organic molecules onto solid surfaces of different kind usually requires the use of solvents (i.e. drop casting, spin coating) adding complexity to the process not only due to the additional step of evaporation of the solvent but also related to the solvent-depending molecular organisation and or the possible presence of impurities. Moreover, insoluble organics cannot be homogeneously deposited by these methodologies. Non-solvent techniques such as chemical/physical vapour deposition or high-vacuum evaporators require of sophisticated devices and/or trained personnel. Alternatively, sublimation is presented as a green methodology which has been widely used in purification or crystallization processes in general chemistry laboratories.

Here we describe a new sublimation system that allows easy and simple deposition of molecules on any type of surfaces and that can be integrated in general laboratories without the need for special equipment.[1,2] The system is completely modular, which allows for the accommodation of substrates of different shapes and sizes, and is designed to minimize the required amount of the organic compounds used in the analysis. Moreover, the molecule-to-substrate distance can be adjusted to fine tune the deposition process. This new sublimation system has been successfully evaluated in the sublimation of curcumin analogues.[3]

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## Integration of curcuminoids into solid state devices for optoelectronic applications

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Curcuminoids (CCmoids) are organic molecules that have been widely studied for biomedical applications, curcumin being the most popular. They exhibit a linear  $\pi$ -conjugated backbone and a remarkable variety of functionalisation at different sites that have allowed their application beyond the biomedical field as a molecular platform for different applications [1]; indeed, they are increasingly considered as building blocks in coordinated CP[4] polymers and MOF[5] metal-organic frameworks. As nanowires, their single-molecule electron transport properties were characterised at room temperature in graphene hybrid devices showing similar conductance values to other small conjugated systems [6]. Here we will present methods developed in our group to integrate new CCmoids of different dimensionality (1D, 2D, 3D) into solid-state devices for applications in the field of optoelectronics. For this purpose, we are developing and characterising both single-molecule and thin-film electronic devices to test target CCmoids systems. The fabrication strategy and the optimization of the molecular functionalization used are discussed along with the results of their electrical characterization [4].

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## Multi-functional Sensing Platform using a Luminescent Material

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In this work we have developed for the first time a multifunctional sensing platform that allows the optical detection of pressure (vacuum), temperature (both crucial parameters in materials science [1]) and excitation power density, using a sensor based on an upconversion inorganic material (NaYF4:Yb<sup>3+</sup>,Er<sup>3+</sup>,Gd<sup>3+</sup>) emitting in the visible range. To measure these parameters without contact, optical methods based on the luminescence of lanthanides, d-block metal ions and organic complexes are usually applied [2]. To develop this sensor, we used the relationship between temperature and luminescence intensity of thermally coupled levels (TCL) of Er<sup>3+</sup>, namely the band intensity ratio (525 nm /550 nm) [3]. We believe that this work can inspire new lines of research that allow the development of materials as multifunctional sensors.



Fig: Concept of thermally-coupled levels from Er<sup>3+</sup>-doped luminescent material.

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## Narrowband perovskite-perovskite photodetectors using vacuum deposition

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Narrowband photodetectors are optoelectronic devices with selective wavelength properties that enable color discrimination. Due to this attractive feature, they are being implemented in fields such as image sensing, optical communication, surveillance systems, etc. The most common method to achieve a narrowband spectral response, is by the combination of optical bandpass filters with broadband photodetectors. However, this approach decreases image sharpness and creates optical interfaces. Here, we report a method using thermal vacuum deposition to obtain narrowband photodetectors by monolithically integrating two perovskites in the device. In particular, we fabricated and characterized a narrowband photodetector following this proof of concept: a multilayer photodiode in a perovskite-perovskite tandem structure. [1] The narrowband spectral response of the photodetectors is determined by the bandgap energy difference of the two perovskite films, exhibiting a full width at half maximum (FWHM) below 85 nm centered in the near infrared and a specific detectivity of 10<sup>12</sup> Jones was achieved, enabling the device to detect weak light signals. Our results demonstrate a new approach to obtain narrowband perovskite photodetectors using vacuum-deposited multilayers.

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## Fluorinated Aliphatic SAM—Efficient P-dopant Replacement for Fully Vacuum Deposited Perovskite Solar Cell

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For commercialization of the perovskite solar cell industry, the most significant viable route is the development of a fully evaporated device that possesses high efficiency and stability and is reproducible. The evolution of industrial Halide perovskite solar cells has been limited by the transport layers. For high-efficiency cells, the use of unstable oxides or dopants is currently inevitable. This improves efficiency yet transfers the device into a feeble structure facing thermal treatments.

In this work, we present a cheap and facile modification of the ITO surface with the use of a self-assembled monolayer (SAM). Recently SAMs got a lot of interest especially the carbazole-containing SAM has been reported to have the function of hole transport material. Here, we demonstrate that with the use of a simple aliphatic fluorinated phosphonic acid as SAM in the ITO interface it is possible to have a fully evaporated solar cell. This gives the advantage of having a commercially adaptable, fully evaporated architecture for future large-area industrialization which is both highly efficient and thermally stable. ITO modification with SAM improves the charge extraction, hence, boosting the PCE to be amongst the highest reported values (close to 19%). Moreover, the system under constant heating at 85C keeps more than 80% of its initial value after 500h.

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# The top-down approach of reducing the {(NH<sub>4</sub>)[Ni(cyclam)][Fe(CN)<sub>6</sub>]·5H<sub>2</sub>O}<sub>n</sub> crystals size

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Coordination systems can exhibit combinations of many desirable properties e.g. transparency, magnetic order, luminescence, or sorption ability and bistability, which allows switching between easily distinguishable states. This multifunctionality and switchability of coordination systems makes them an interesting alternative for classical materials used in electronic devices. However, coordination systems are usually obtained as crystals, which are often brittle and difficult in mechanical processing, easy to destroy by even mild chemical conditions, which may result in the loss of desired properties.

The preparation of coordination systems in robust form keeping their original behavior is necessary for their potential application in modern devices. The promising solution seems to be formation of thin films or nanocomposites based on switchable coordination compounds embedded in an organic polymer matrix. Such nanocomposites could combine multi-functionality of the chosen material with favorable mechanical properties of the organic polymer.

The  $\{(NH_4)[Ni(cyclam)][Fe(CN)_6]\cdot 5H_2O\}_n$  bimetallic chain is a perfect candidate for a three-way switchable sensor reacting to temperature and humidity changes as well as mechanical stress. It shows thermally induced metal-to-metal charge transfer in the Nill/III-FeIII/II redox pair with hysteretic behavior in the room temperature range, which can be switched off by dehydration [1]. In order to exploit the potential of this compound, it is important to prepare it in the form of films or composites. The crucial step in this process and the purpose of this work is finding the optimum way to reduce the size of the crystals to nanometric scale. Since it is impossible to obtain the compound in the form of nanoparticles in solution methods, we apply the top-down approach of reducing the crystal size by milling, ultrasonic homogenization, or subjecting the compound to repeated solid state phase transitions (Figure 1).



Figure 1. SEM microphotographs of the {(NH<sub>4</sub>)[Ni(cyclam)][Fe(CN)<sub>6</sub>]·5H<sub>2</sub>O}<sub>n</sub> particles after reducing the crystal size

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## A ROBUST AND PREDICTIVE PLATFORM FOR THE CHARACTERIZATION OF NEXT-GENERATION POLYPEPTIDE-DRUG CONJUGATES

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The exhaustive characterization of polypeptide-drug conjugates (PDCs) will permit the optimization of drug release kinetics and the improvement of drug bioavailability to enhance translation from bench to bedside [1-3]. Thus, there is a high need for a robust and predictive platform to characterize next-generation PDCs, in particular, to better design polypeptide-drug liking chemistries. In this study, we highlighted the importance of implementing appropriate, accurate, reproducible, and sensitive analytical methods from the beginning and throughout the PDCs design process to yield PDCs with an adequate therapeutic output.

Therefore, we employed the design of experiments (DoE), a quality-by-design approach, to obtain an internal database of liquid chromatography-mass spectrometry (LC-MS) methods for quantitative determination of selected anticancer drugs used in our PDCs design. In order to better understand the biological fate of PDCs, first, cell studies should be performed. We will, then, implement the DoE developed LC-MS methods in the *in vitro* drug release studies after optimization of the sample preparation process for the extraction of the selected anticancer drugs from cell medium and cancer cells. All the developed methodologies were validated with a model polyglutamic acid (PGA) navitoclax anticancer conjugate including a disulfide self-immolative linker (PGA-SS-Ph-NVTX). This data shows how an appropriate analytical protocol is an invaluable tool for uncovering PDCs fate in biological environments.

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## Green Synthesis of Silver Nanoparticles with Biological Activity

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## Abstract:

Metal nanoparticles with antimicrobial activity have long history of wonders. The large number of particles that can be made and the high surface area to volume ratio allows nanoparticles to be effective in very small amounts (Zain, 2014)<sup>[1]</sup>. Currently working on silver nanoparticles, as per previous research work it is concluded that stable sliver nanoparticles were synthesized by using chitosan, which act both as reducing and stabilizing agent. (Maragoni Venkatesham, 2014)<sup>[2]</sup>. We have prepared Silver nanoparticles by using a comercial chitosan sample (Chitopharm S) and a chitosan derivative (Chitosan Sulfate) both as reducing agent and stabilizer. Polymer solutions were produced by dissolving different amount of polymer (4mg, 5mg, 10mg) in 1 mL of acetic acid solution (1% w/v) or water. Samples were stirred overnigth on magnetic stirrer. Freshly prepared silver nitrate solutions (5mM in water) were added to the polymer solution (200 µL of silver solution per mL of polymer solution) and the mixture was vorterex for 3-4 seconds. Control sample was produced by adding the silver nitrate solution to water. The mixtures were placed at 90°C for over night to get silver particles formed. A curve between 350 to 450 nm shows optimal absorbance of light by silver nanoparticles also slight vellowish color indicates the formation of silver nanoparticles [Fig.1]. The synthesized silver nanoparticles were characterized by using UV-Vis Spectroscopy. Analysed between 200 nm and 700 nm in order to observe the presence of silver surface plasmon resonance (SPR) around 400 nm. Samples were also characterized with a zeta sizer analyser from malvern in terms of size and zeta potential.

We are currently studing the effect of the influence of different parameters such as time, change of concentration of silver nitrate and concentration of chitosan on the formation, later we will also studied about stability of silver nanoparticles over long (30 to 40 days) period with same conditions.



Figure 1: The ultraviolet-visible (UV-vis) spectra of silver nanoparticles (AgNPs) with and without chitosan (CH)

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## Characterization of nanoparticle diffusion in a tumor-on-a-chip device

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Recent advances in nanomedicine have provided hope for cancer detection, prevention and treatment. Although the enhanced permeability and retention (EPR) effect constitutes a key phenomenon to selectively deliver nanomedicines to tumors, it does not enable a homogenous delivery of nanomedicines to all tumor regions in sufficient quantities [1]. In tumor, the ideal delivery of nanomedicines is limited by an elevated interstitial fluid pressure, abnormal tumor vasculature, dense tumor extracellular matrix and elevated solid stress [2]. Therefore, understanding nanomedicines diffusion inside the extracellular matrix (ECM) is key to achieve homogeneous delivery and, as a result, an improvement in therapeutic efficacy [3].



Figure 1. Schematic representation of double-channel microfluidic tumor-on-a-chip device, where the solid stress in the extracellular matrix is recreated. *Figure created with BioRender.com*.

Tumor-on-a-chip devices represent ideal platforms to recreate *in vitro* the physiological microenvironment of a tumor, allowing the study of nanomedicines diffusion [4]. It is a double-channel microfluidic device, one channel is an artificial blood microvessel and the other represents a tumoral cavity, where different extracellular matrices are introduced, such as collagen gels and Corning<sup>™</sup> Matrigel<sup>™</sup>, see Figure 1. Thanks to these properties, it is possible to recreate tumor solid stress, in order to study its effect on nanoparticles diffusion. In this device, the diffusion mechanism of nanoparticles is monitored by fluorescence microscopy, leading to the performance of permeability measurements.

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## **Characterization Of Two-Dimensional Perovskites**

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Abstract body: single spaced paragraph. End spacing is 6pt after. Font Arial size 11 pt. Perovskites had been used for a long time due to its properties and the magnifical stability of its two-dimension (2D) structure compared to the three-dimension (3D) one. Despite 3D-perovskites having plenty of useful qualities, its instability made them less useful for different purposes. 3D hybrid perovskites have an ABX3 structure, where typically A is an organic cation (MA+ = methylammonium), B is a metal cation (Pb2+ or Sn2+) and X is a halide (CI-, Br- or I-) which leads to an octahedral structure with the halogen element situated in the corners.[1]

Through the use of different techniques such as spectroscopy, photoluminescence or fluorescence among others it's possible to characterize the main properties of perovskite, opening the way to its use for the manufacture of solar panels.



Perovskite flake photoluminescence seen under a microscope.

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## Chemically robust metal-organic framework based biocomposites for their use in biotechnological processes.

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Metal-organic frameworks (MOFs) have emerged as a promising material for enzyme encapsulation due to their high porosity and tunable structure [1]. The in situ encapsulation of enzymes in MOFs can protect them from harsh environments, enhancing their stability, activity, and selectivity, and therefore having an impact on their biotechnological uses.

Among the plausible MOF structures to be used as protective skeleton, Zirconium-based MOFs are particularly interesting due to their exceptional stability and optimal biocompatibility. Despite this, the in situ encapsulation of enzymes in zirconium MOFs remains a challenge, mainly due to the difficulty in obtaining a compatible synthetic route that preserves enzyme activity. In this sense, further research is needed to optimize the in situ encapsulation process.

Herein, we will show our advances in the encapsulation of lipase, an enzyme that catalyzes the breakdown of fats into fatty acids and glycerol, into robust zirconium-based MOFs. Our final goal will be to evaluate the activity of these enzymes in bioreactors for the production of biodiesel [2].

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## **Engineering Chiral Porosity in Metal-Organic Frameworks**

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Metal-Organic Frameworks (MOFs) are a novel family of nanomaterials in which metal ions or clusters (nodes) are joined together using organic molecules (ligands) to make crystalline porous frameworks [1]. One of their main advantages is the possibility of functionalizing their structures for specific applications. To achieve this, postsynthetic modifications (PSM) of MOFs have gained significant interest due to their simplicity and non-invasive effect on the crystallinity and porosity of the materials [2].

In this work, we describe two completely different approaches to graft chiral natural amino acids and peptides into MOFs: one node-directed via vacant-site chemistry and one ligand-directed via biorthogonal chemistry. We discuss the primary differences and advantages of each method. Targeted engineering of chiral voids within porous frameworks, not limited to guest inclusion, is a powerful tool to enable these solids to recognize and discriminate chiral guests for catalysis and separation purposes [3].



**Figure 1:** Graphical abstract. On the left, amino acids are introduced into NU-1000 into the metal nodes. On the right, amino acids are introduced into UiO-68-TZDC into the organic ligands.

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## Manufacture and characterization of cellular materials with guest phases for applications in medical implantology

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Guefoams are a family of materials with open-pored cellular structures that contain functional phases (guest phases) in their cavities that give the material a wide range of applications, including implants in bone cavitations [1-3]. The objective of the present study was to manufacture and characterize Guefoams materials of magnesium matrix and activated alumina guest phase that act as a drug-releasing agent for future applications in bone implantology. The structural matrix has an oxide layer obtained by heat treatment, while the guest phase contains an adsorbed antibiotic compound. The results have shown that the structural matrix of the Guefoams has cellular capacity, while the presence of the host phase provides it with a great antibacterial capacity, making these materials suitable candidates for implantology.

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## Mechanically Interlocked Carbon Nanotubes: Functionalization and Separation of Single-Walled Carbon Nanotubes

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Single-walled carbon nanotubes (SWNTs) have attracted significant interest due to their unique properties, such as an extremely high Young's modulus and ballistic charge transport in metallic SWNTs. SWNTs were envisioned as the material of the future for many applications, from stronger composite materials to ultrasensitive sensors. However, their implementation into marketable technologies has been hindered by two main problems: their tendency to aggregate and their poor interaction with other materials. For these reasons, obtaining electronically monodisperse SWNT samples is still a big challenge. Thus, chemical modification of SWNTs has been used to address these issues.

In 2012 we reported a new approach to functionalize SWNTs and obtain materials known as mechanically interlocked nanotubes (MINTs). MINTs are formed by attaching macrocycles to SWNTs via a mechanical bond, which offers the advantages of both covalent and non-covalent functionalization: very stable products without altering the structure of the SWNTs.<sup>1</sup>

In this study, we focused on two main aspects of MINTs. First, we synthesized Ushaped molecules from pyrene for further functionalization of SWNTs through a ringclosing metathesis reaction. The resulting U-shapes and MINTs were structurally characterized using different techniques, such as <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS, and spectroscopic thermogravimetric techniques.

Second, we separated non-functionalized carbon nanotubes from MINTs using an allyl dextran-based size-exclusion gel and different surfactants, such as sodium dodecyl sulfate (SDS) and sodium cholate, to disperse, extract and separate the carbon nanotubes. The separation conditions were optimized by varying the surfactant concentration. Positive results were obtained, as evidenced by the UV-Vis and PLE spectra of the fractions collected from the column.



Covalent: stability but structural change

MINTs: stability and structural integrity Figure 1. Mechanically interlocked carbon nanotube<sup>1</sup>

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## Optical contrast identification of atomically thin-layers of the Van der Waals ferromagnet Fe<sub>3</sub>GeTe<sub>2</sub>

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Two-dimensional (2D) materials exhibit specific outstanding properties and provide a platform for a wide range of applications such as sensing, data storage or spintronics, just to mention some. [1] Following the discovery of graphene, 2D magnetic materials have been recently isolated, as exemplified in monolayer Crl<sub>3</sub> [2]. Here we focus on the Van der Waals ferromagnet Fe<sub>3</sub>GeTe<sub>2</sub> with high Curie Temperature (T<sub>c</sub> = 200 K) and its metallic behavior (in contrast with Crl<sub>3</sub>). [3] A key ingredient for the fabrication of 2D devices is the reliable identification of atomically-thin layers with optical contrast being one of the most suitable methods. Thus, atomically-thin layers of Fe<sub>3</sub>GeTe<sub>2</sub> are mechanically exfoliated inside an argon glove-box in order to quantify their optical contrast and correlate it with the thickness determined by atomic force microscopy. In addition, we consider the time degradation of this material in air by optical contrast and Raman spectroscopy. [4]



Figure 1 : Optical microscopy images without filter (a), with 550 nm filter (b) and its corresponding experimental optical contrast (c). Scale bar : 10 µm and calibration curve for thin layers of Fe<sub>3</sub>GeTe<sub>2</sub> on 285 nm SiO<sub>2</sub>/Si substrates under illumination with different wavelengths (panel d)

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## Preparation of long modified DNA with tunable properties.

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DNA molecules have demonstrated to have a great potential in nanostructures thanks to the self-assembly of the nucleotides [1]. However, biological molecules, such as DNA, have compromised conductivity, thus, the development of new devices with electronic properties remains a challenge nowadays [2]. The aim of this project is to produce long modified DNA structures (e.g., >5000 bp, >1700 nm) with novel properties (e.g., conductivity) for nanotechnological applications. This approach is based on the incorporation of 5-vinyl-2'-deoxyuridine nucleoside into the DNA, which will be pursued following two strategies. One implies an enzymatic process based on PCR, and the other uses bacteria. Once the DNA has been modified, the vinyl derivative will be reacted with a tetrazine group containing a molecule of interest through a Diels-Alder reaction. The final DNA structures containing the desired molecules will be characterized by absorbance, fluorescence, and SPM techniques.



Figure 1. Representation of the in vivo strategy planned for the preparation of modified long DNA structures.

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## Programming Amino Acids for controlling Framework Flexibility

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Metal-organic frameworks (MOFs) are a family of porous materials built from the controllable assembly of metal ions or clusters with organic linkers [1]. Flexible MOFs are a specific type of these frameworks that can exhibit dynamic structural changes in response to external stimuli, such as temperature, pressure, or guest loading [2]. These structural changes can result in modifications to the pore size and shape, surface area, and guest uptake capacity, making them particularly useful in gas storage, separation, and sensing applications.

In this work, we present the use of synthetic amino acids, that overcome the stability limitations imposed by their proteogenic counterparts and are well adapted for the systematic assembly of flexible pores. The intrinsic flexibility and side chain chemistry of these amino acids is used to endow the resulting material with the ability to adapt its structure and recognize external guests.



Figure 1. On the top, the organic linker with the desire modifications. On the bottom, a representation of our hypothetical material adapting its size to a rigid guest.

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## Synthesis of nanoparticles for cell culture and microscopy studies

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The main objective of this study is to synthesize biocompatible colloidal nanoparticles (NPs) that can be further used as nanothermomethers in biological media. [1] Their role as nanothermometers results from the change of their photoluminescence (PL) response with temperature. We focus on silver sulphide (Ag<sub>2</sub>S)-based NPs synthesized in several steps by means of a so-called "hot injection method" [2]. A transmission electron microscopy (TEM) image of these NPs is shown in **Figure 1**. The biocompatibility is provided by the treatment of the NPs with a modified polyisobutylene-alt-maleic anhydride compound, a well-known amphiphilic block copolymer. [3] On-going studies evidence a good colloidal stability in water and excellent PL signal. Further cell-culture studies and microscopic inspections are planned.



Figure 1.- TEM image of Ag<sub>2</sub>S-based colloidal NPs

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## Toward the control of the membrane insertion of a pH-sensitive peptide with light

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## Abstract

The pH Low Insertion Peptide (pHLIP), and its derivatives, are amphipathic peptides that interact with lipidic membranes in a pH-dependent manner. At neutral pH pHLIP binds to the membrane interface but at low pH conditions it inserts in membranes as a transmembrane alpha helix, with an apparent pKa of ~6. In this process, its C-terminus of pHLIP traverses the membrane, an opportunity to create drug delivery systems that target acid extracellular environments, such as those of cancerous cells [1].

The structural changes of pHLIP at the beginning and end stages of insertion have been characterized by conducting static spectroscopic experiments as a function of the pH [2]. However, the requirement to change the pH of the medium to induce the insertion of pHLIP has limited such studies, both in structural detail and temporal resolution.

Our strategy to trigger the insertion of pHLIP is to use light instead of pH changes. To do so, we will use membranes containing a mixture of the standard lipid POPC and the photo-switchable lipid azo-PC [3]. This will allow for increasing the fluidity of the membrane by trans-to-cis photo isomerization of azo-PC, which we expect to reduce the pKa for the membrane insertion of pHLIP [3]. This will allow us to follow the insertion of pHLIP with great detail without the need to change the pH, with the practical benefits of using light as a trigger.

As a starting point, we have determined the pKa for the insertion of pHLIP into POPC membrane by following changes in the emission fluorescence of its two tryptophan residues as a function of the pH, as described before [2]. Next, we plan to use the same strategy to determine the pKa for insertion in POPC/azoPC membranes, both for its trans (dark) and cis (light) forms. Differences in the pKa for insertion induced by light will be used afterward to trigger the insertion of pHLIP at a fixed pH value. Such technical advantage will allow for experiments currently unfeasible, increasing our understanding of how pHLIP inserts into membranes.

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## Development of a second generation of extended triphenylamine-based fluorescent ligands for G-Quadruplex DNA detection and visualisation

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Among various alternative DNA structures, G-Quadruplex (G4) DNAs have attracted considerable interest over the last two decades. These non-canonical secondary DNA structures are formed under physiological conditions by the self-assembly of guanine-rich nucleic acid sequences and predominantly exist in biologically important regions such as gene promoters or telomeres, which are involved in crucial biological processes, including DNA replication, gene transcription and genome maintenance. Evidence suggests their pivotal role in neurological diseases, ageing processes and cancer<sup>1</sup>. However, the exact nature of their biological significance is still poorly understood. Consequently, these G4 structures have been proposed as potential targets for therapeutic intervention and in order to unravel the biological processes in which G4s are involved, several strategies have emerged such as antibodies and small optical probes<sup>2-3</sup>.

In this line, our team has launched a project of G4 probes based on the triphenylamine scaffold and found two ligands with strong interaction and selectivity for G4 structures<sup>4-5</sup>. Herein, we present our synthetic efforts to develop a second generation of extended triphenylamine-based molecules with an extended aromatic core in order to enhance the photophysical features for bioimaging while maintaining excellent binding abilities for G4s. In addition to the already reported NBTE<sup>6</sup> (a molecule formed by a triphenylamine core with three ethylenic chains in *para* position), we have prepared its methylated version with the amine in *para* (TPPA-4pyrM) and *meta* (TPPA-3pyrM) position.

A range of biophysical assays (FRET melting, fluorescence spectroscopy and molecular modelling) has been used to characterize the binding mode of action. Overall, our results point out the importance of the organic core, the extended aromatic scaffold and the aliphatic conjugation to obtain strong G4 binders with fluorescent emission properties to be applied as optical probes for detecting G4 structures.

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## High elasticity and strength of ultra-thin metallic transition metal dichalcogenides

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Mechanical properties of transition metal dichalcogenides (TMDCs) are relevant to their prospective applications in flexible electronics. So far, the focus has been on the semiconducting TMDCs, mostly  $MoX_2$  and  $WX_2$  (X = S, Se) due to their potential in optoelectronics [1]. A comprehensive understanding of the elastic properties of metallic TMDCs is needed to complement the semiconducting TMDCs in flexible optoelectronics. Thus, mechanical testing of metallic TMDCs is pertinent to the realization of the applications. Here, we report on the atomic force microscopy-based nano-indentation measurements on ultra-thin 2H-TaS<sub>2</sub> crystals to elucidate the stretching and breaking of the metallic TMDCs. We explored the elastic properties of 2H-TaS<sub>2</sub> at different thicknesses ranging from 3.5 nm to 12.6 nm and find that the Young's modulus is independent of the thickness at a value of 85.9 ± 10.6 GPa, which is lower than the semiconducting TMDCs reported so far. We determined the breaking strength as 5.07 ± 0.10 GPa which is 6% of the Young's modulus. This value is comparable to that of other TMDCs. We used ab initio calculations to provide an insight into the high elasticity measured in 2H-TaS<sub>2</sub>. We also performed measurements on a small number of 1T-TaTe<sub>2</sub>, 3R-NbS<sub>2</sub> and 1T-NbTe<sub>2</sub> samples and extended our ab initio calculations to these materials to gain a deeper understanding on the elastic and breaking properties of metallic TMDCs. This work illustrates that the studied metallic TMDCs are suitable candidates to be used as additives in composites as functional and structural elements and for flexible conductive electronic devices.



Figure:1 Schematic of the indentation setup

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## Localized Strain by Spin Crossover in Van der Waals Heterostructure

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Van der Waals Heterostructures (vdWHs) present many possibilities for engineering new materials with different interesting properties and functionalities[1]. Here, we present a novel heterostructure composed of an exfoliated spin-crossover crystal and a twodimensional (2D) semiconductor, CrSBr. We choose CrSBr due to its rich excitonic behaviour, vdW stacked structure, magnetic transitions, and air stability[2]. On the other hand, spin crossover (SCO) materials exhibit a bistable spin transition in presence of external stimuli, which leads to major effects on their electronic, magnetic, optical, and mechanical properties[3]. By using the change in the volume that comes with the spin transition of the SCO crystal, a mechanical strain is applied on the CrSBr forming the heterostructure. This strain effect affects the CrSBr photoluminescence (PL) emission on its spectral width, energy, and intensity. With this, we can study the spin transition optically through the strain effects over the CrSBr PL. In addition, we show how these effects in the PL are located in the area of the 2D flake containing the heterostructure. In this way, these heterostructures have the potential to create novel optoelectronic devices and nanostructures with high tunability and unique optical properties.



Figure 1. A) Optical microscope image of the heterostructure. B) Integrated µPL intensity mapping of the heterostructure at 100 K. C) PL spectra taken at different spots of the sample marked in (B).

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## QUANTIFICATION OF ULTRA-TRACE GRAPHENE OXIDE IN REAL WATER SAMPLES BY SERS

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The use of graphene oxide (GO) increases in many products due to its vast number of excellent properties. However, this extensive use in real-world applications has increased their potential release into the environment. To evaluate their possible health and ecological risks, there is a need for analytical methods that can quantify these materials at very low concentrations in environmental media such as water. The selected analytical technique must allow differentiation between carbon nanomaterials and other carbon compounds present in real water samples. For this reason, Raman spectroscopy is applied as a perfect option, specifically its most innovative variant, surface-enhanced Raman scattering (SERS). This technique allows to detect and quantify GO with high selectivity and sensitivity. This method is able to detect GO in the concentration range of 0.1–10.0 ppb. Using SERS, in this work was achieved a quantification method of GO at trace levels [1], 0.1 ng mL-1, which is lower than the predicted concentrations for graphene in effluent water reported to date. And the recoveries obtained ranged from 95.66% to 100.47%. This methodology has been successfully applied to samples of real filtered water with GO filters and release of GO was excluded [2].



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## A user-friendly DFT computational tool to get insight into quantum and spin transport in molecular junctions.

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A single molecular junction usually is formed by two metal leads and a molecule trap between them. In studies related to electron and spin transport, the relative orientation of the molecule in relation to the electrodes plays a critical role. This relationship of transport and molecular orientation can be studied through Density Functional Theory (DFT) calculations.

Advance DFT codes like ANT.G [1] or TranSIESTA [2] help us compute quantum effects such as electronic and spin transport or density of states in molecular junctions. However, they don't have any easy interface. Here we show our novel tool for manipulating electrodes and molecules and generate inputs for ANT.G.



Figure 1. Interface of the tool. The left panel holds the controls for editing the output. On the right a realtime interactive 3D plot of the input.

The tool is a user-friendly interface to edit and change in real time the positions of electrodes and molecules in the junction. The ease to create customs inputs for Molecular Dynamics or DFT electronic and spin transport calculations have given us the opportunity to do quick and vast analysis of a wide range of molecules and properties, like the ones made on common organic solvents [3] or some other computations and comparisons that will be shown in the presentation.

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## Synthesis and characterization of the optical properties of SCO nanomaterials in the IR for their integration into nanophotonic devices

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The development of low-energy nanophotonic devices for new photonic and optoelectronic applications depends on the capability to control the light in the nanoscale in the photonic chips [1]. In this context, the integration of molecular spin crossover (SCO) nanomaterials [2] in the Si photonic platform can provide unique and tunable properties which can be chemically engineered to obtain bistability at room temperature (RT) with hysteretic behaviour. This represents the main feature to develop non-volatile response and low-power operation [3]. During the development of this work, two types of nanoparticles (NPs) [4] that present SCO behaviour have been synthesized and studied. These two types of SCO NPs present optical bistability near RT with different transition temperature ranges. Their characterization has been divided in morphological, magnetic and optical. Morphological characterization has been developed with DLS to prove that shape and size are as expected. Magnetic characterization was applied with SQUID to characterize the transition temperature ranges. Once the morphological and magnetic characterization was completed, the SCO NPs were integrated in a Poly(methyl methacrylate) (PMMA) matrix and deposited on a gold substrate to perform the optical characterization in the IR. Further studies as well as the fabrication of hybrid SCO based photonic structures in photonic platforms will be performed to develop in the future low-power nanophotonic switches, as well as reconfigurable metasurfaces.



**Figure 1.** Reconfigurable surfaces prototype device based in SCO materials placed in both states (High spin(HS) and Low Spin(LS)).

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## Theoretical study of Spin Transition Complexes and their application in Molecular Spintronics

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Spin Crossover (SCO) molecules<sup>1</sup> are molecular switches proposed as active Spintronic elements due to the particular interplay between their conductive and magnetic properties. Particularly, sublimable spin switchable molecules are easier to process as integrated nanocomponents within a new class of spintronic devices providing features that cannot be otherwise obtained with classical inorganic materials. In this work, we study a common SCO molecule<sup>2-3</sup>, [Fe(3,5-diMepyrz)2] (3,5-diMepyrz = 3,5-dimethylpyrazolylborate) when deposited onto metallic surfaces. By comparing the geometrical and electronic structure in the different configurations, we show that, in unbiased conditions, the electronic molecular orbitals responsible for the spin switching are dramatically altered by the interaction with a metallic surface. In this aspect, we offer new insights about how the magnetic nature of the substrate is able to modify or even suppress the spin switching.



Figure 1. Molecular structure of [Fe(3,5-diMepyrz)2] (3,5-diMepyrz = 3,5-dimethylpyrazolylborate).

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## Breathing spin crossover coordination framework with elastic frustration controlled by guest molecule adsorption

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Spin crossover (SCO) phenomenon is controlled by physical stimuli such as temperature, pressure or light. SCO is mainly governed by the local ligand field strength and is strongly affected by the elasticity of the crystal lattice in the case of solid state systems. In some cases, the removal or insertion of guest molecules may lead to significant changes in the cooperativity of SCO or even the appearance of elastic frustration.

We have prepared a three-dimensional coordination framework {[Fe<sup>II</sup>(4-CNpy)<sub>4</sub>]<sub>2</sub>[W<sup>IV</sup>(CN)<sub>8</sub>]·4H<sub>2</sub>O}<sub>n</sub> (4CNpy = 4-cyanopyridine) belonging to the Fe<sup>II</sup>-pyR-[M<sup>IV</sup>(CN<sub>8</sub>)] family (pyR = pyridine derivative). This compound shows thermally-induced partial SCO with symptoms of elastic frustration below 260 K, as well as light induced excited spin state trapping (LIESST) effect upon 638 nm light irradiation at 10 K. The compound can be dehydrated in a single-crystal-to-single-crystal fashion, yielding the anhydrous phase {[Fe<sup>II</sup>(4-CNpy)<sub>4</sub>]<sub>2</sub>[W<sup>IV</sup>(CN)<sub>8</sub>]<sub>n</sub> which was also studied using X-ray diffraction. The water-free phase shows no sign of elastic frustration and displays almost complete SCO with  $T_{1/2} = 91$  K. Despite drastically different thermal SCO behaviour, both phases show very similar photomagnetic properties, with almost identical  $T_{\text{LIESST}}$  of 57-59 K. Moreover, the CO<sub>2</sub> adsorption experiment performed on the anhydrous phase have shown the so-called 'gate-opening' effect which stabilizes the high spin state of the Fe<sup>II</sup> centers in the investigated temperature range 2-300 K.



**Figure 1** Guest molecule (H<sub>2</sub>O and CO<sub>2</sub>) adsorption controls the elastic frustration and the LIESST behaviour of the SCO frameworks. Pink and yellow balls- Fe(II) atoms, arrows- spins.

## Caged Proton-Transfer Dyes within MOFs for Luminescence Sensing of Acid and base Vapors

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Luminescent Metal-Organic Frameworks (LMOFs) are porous crystalline material with the ability of emitting light and they have become one of the most popular luminescent nanomaterials over the last decade [1]. On the other hand, molecules experiencing an Excited-State Proton Transfer phenomenon (PT-dyes) have been extensively investigated due to their excellent luminescent properties, including their potential to detect anions or cations.[2] Hence, owing to the LMOF porosity, there is a great opportunity to incorporate PT-dyes within the MOFs, aiming to exploit the luminescence of these materials to detect vapours of acid or base chemicals through changes in their fluorescence.

Thus, herein we present the synthesis, structural characterization, and steady-state properties of two distinct PT-dyes (8-hydroxypyrene-1,3,6-trisulfonic acid trisodium salt (HPTS), and 3-hydroxyflavone (3-HF)) encapsulated within the pores of two well-known MOFs, ZIF-8 and UiO-66 (**Figure 1a**). Both molecules are in the anionic form when encapsulated in ZIF-8, while when encapsulated in UiO-66 they are in the enol form. Hence when their interaction with HCI (acid) or  $Et_3N$  (base) vapours induces a change in the emission colour of these materials (**Figure 1b**). We will also discuss the results using time-resolved emission spectroscopy providing details on the involved mechanism of sensing.



Figure 1. A) Representation of HPTS encapsulated within ZIF-8, and chemical structures of protonated and anionic HPTS tautomers. B) Emission spectra of HPTS@ZIF-8 in absence and in presence (incremental times of exposition) of HCI vapor. The inset shows photos of HPTS@ZIF-8 powder before and after exposing (30 min) to HCI under UV (365 nm).

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## Magnon straintronics in 2D materials

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2D magnetic materials expanded the scope of material science to design devices that can offer a plethora of opportunities [1]. One of the most important groups of 2D magnetic materials is CrX<sub>3</sub> (X: Cl, Br, I) where in particular Crl<sub>3</sub> was the first 2D ferromagnet in the monolayer limit [1]. Another promising group of 2D magnetic materials is the MPS<sub>3</sub> (M: Fe, Ni, Co, Mn) family, formed by van der Waals materials with excellent electronic and optical properties [2-5]. Despite all these properties make 2D magnets very interesting by themselves, the magnetism present in these materials is wide and yet not well understood, giving rise to exotic phenomena. Herein we present a theoretical methodology to analyse 2D materials, based in DFT calculations, Wannier Hamiltonians and Green functions. Using these techniques, the magnetic and exchange properties can be resolved in terms of chemical orbitals and improved with strain simulations that result in an increase of Curie temperatures and magnon propagation along the 2D materials, [6,7] thus exploring alternative platforms for spintronic devices.



Figure: Strain in 2D magnets: Exchange interactions, Curie temperature and magnons modes.

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## Molecular intermetallics with unsupported 4f-3d metal-metal bonds as candidates for high-temperature SMMs

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Currently many paths are explored to obtain high-temperature single molecule magnets (HT-SMMs). The one presented in this work is to build intermetallic complexes mimicking the first coordination sphere of Sm centres present in commercial SmCo<sub>5</sub> permanent magnets [1]. This approach aims at designing direct exchange interactions between lanthanide and transition metal ions within a single molecule. It is hypothesized that direct exchange interactions can suppress QTM in molecular nanomagnets [2]. Here, we present the first attempt towards molecular intermetallic systems where the coordination geometry and the ground state of the electron density of the central Ln ion are shaped solely by transition metals acting as the only donor atoms [3].

Within this vein of research, we have synthesized and characterized two intermetallic complexes with direct lanthanide-transition metal bonds:  $Er^{III}(Re^{I}Cp_{2})_{3}$  (**ErRe**<sub>3</sub>, Fig. 1)[4] and its ytterbium(III) analogue Yb<sup>III</sup>(Re^{I}Cp\_{2})\_{3} (**YbRe**<sub>3</sub>) (Cp = cyclopentadienyl anion). Crystal structures of both complexes are isomorphous. They crystalize in trigonal crystal system (*R*-3 space group). Lanthanide ion is solely coordinated by three diamagnetic Re(I) ions in a trigonal planar fashion. Measurements of their magnetic properties have been conducted and it showed that  $ErRe_3$  is a very good SMM with pinched magnetic hysteresis loop that can be observed up to 7.2 K (at 2.2 mTs<sup>-1</sup> magnetic sweep rate). It exhibits slow magnetic relaxation with effective energy barrier for the magnetization reversal of 314(5) K (from experimental data) and 363 K (from theoretical calculations). However, for the YbRe<sub>3</sub> compound the magnetic properties dramatically change with no observation of the slow magnetic relaxation.

Now for the hard question: what is the reason for such a vast change in the magnetic properties between  $ErRe_3$  and  $YbRe_3$ ?



Figure 1. Single-crystal structural model of the ErRe3 complex.

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## NBD/QC single molecule electronic switches, effect of chemical anchor groups

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Decreasing the dimensions of semiconductor devices is one of the most discussed topics in the field of nanotechnology. Single molecule devices could provide a new pathway for the miniaturization of electronic devices. Single molecule electronics are used to fabricate electronic devices with various functions such as switching, transistors, and molecular diodes. In this project we aim to find new candidates for molecule switch. We report both experimental and computational study of three different thiol substituted norbornadiene (NBD) molecules to examine the effect of anchor groups attached to gold electrodes (Figure1) using for the first time mechanically controlled break junction technique (MCBJ) techniques to study the NBD system. [1,2]



Figure 1: single molecule electronics set-up

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## Polar Mn(II)-based multifunctional molecular material exhibiting humiditysensitive luminescent, magnetic, and electrical properties

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Over the last years molecule-based materials based on coordination compounds incorporating earth-abundant metals, including those based on *d*-block metal complexes such as manganese, chromium, iron, and cobalt, have aroused growing interest because of their potential in substituting expensive heavy metals for applications in light-emitting diodes (LEDs), optical sensing, optical storage, as well as for their broad set of accessible magnetic, magneto-optical and magneto-chiral functionalities [1-6].

In this work, we present a novel multifunctional molecular material based on Mn(II) complexes with Me-dppmO<sub>2</sub> (bis(diphenylphosphino)-1,1-ethane dioxide) ligands. It is an organic-inorganic salt (1) that crystallizes in the polar *Cc* space group and exhibits the SHG phenomenon and a series of humidity-sensitive physical properties, including strong yellow (maximum at ca. 560 nm) photoluminescence in the solid state at room temperature (Figure 1), slow magnetic relaxation effects below 10 K, and the dielectric relaxation switchable by the presence of water molecules of crystallization in the material. The humidity sensing potential of this system, considered from the viewpoints of its optical, magnetic, and electrical properties, is discussed.



Figure 1. Room-temperature SHG intensity power dependence with the wavelength dependence in the inset (left), the crystal structure packing of 1 alongside the **a** axis (center), and the relative humidity-dependent solid-state photoluminescence spectra at room temperature (right).

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## SHG-active luminescent thermometers from chiral dicyanidoiridates(III)

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Due to strong and controllable emission that ranges from visible to NIR spectrum, some transition metal complexes such as cyclometalated iridium(III) complexes are useful molecular building blocks for the formation of novel optical materials.[1] They were also investigated for advanced photonic applications related to chirality-related phenomena like circularly polarized luminescence (CPL), while the relative cyanido transition metal complexes were employed for magneto-chiral dichroism (MChD) or magnetization-induced second harmonic generation (MSHG).[2,3,4] In this regard, we focus on the non-trivial coupling of organometallic and cyanide chemistry to produce a novel class of chiral luminescent dicyanidoiridate(III) complexes used for optical functionalities, e.g., luminescent thermometry.[5] In this work, we present the class of molecular materials that are based on dicyanidoiridate(III) complexes with a chiral (R,R)-pinppy ligand. They range from ionic salts to coordination polymers. Materials that have been obtained combine the SHG effect with strong photoluminescence of a ligand-to-metal charge transfer character, and unique luminescent thermometry.



**Figure 1.** (from left to right) Crystal structure of the prepared dicyanidoiridate(III) molecular building block used for the coordination compounds **1** and **2**, temperature-dependent emission spectra together with the thermometric parameter for **2**, the power dependence of the SHG effect for **1** and **2**, and DFT-calculated differential electron density map for the first emissive state of the Ir(III) complex.

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## Tuning interparticle interactions in closely packed iron oxide nanoparticle assemblies

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Magnetic nanoparticle assemblies show individual-like and/or collective-like properties depending on the strength of the interparticle interactions compared to the single-particle anisotropy, factors which determine their magnetic performance [1]. Dense assemblies of iron oxide-based nanoparticles are excellent systems by which to study the role of these factors [2]. Here, we present a magnetic characterization of a series of closepacked assemblies of 5-nm-diameter maghemite  $(\gamma$ -Fe<sub>2</sub>O<sub>3</sub>) particles at increasingly higher particle packing fractions. The different assemblies were obtained by die compaction of nanoparticles after being subjected to a partial removal of the initiallycomplete oleic acid (OA) shells. We harvest different indicators of interparticle interaction strength from various SQUID magnetometry techniques: namely, peak temperature in ZFC curves (T<sub>max</sub>) and dip depths associated to ZFC memory effects and to remanence magnetization ( $\Delta M$ ) curves. These indicators are found to correlate along the series, all pointing to a rise in the interparticle interaction strength. However, the relative size of the increase in  $T_{max}$  is an order of magnitude larger than that in the packing fraction, indicating that the rise in interaction strength is not due alone to a rise in magnetic dipolar strength [3]. Supported by SAXS, we suggest that the OA removal leads to uncoated surface regions of particles, which come into direct contact. Furthermore, we suggest that this direct contact, together with the particles' lack of surface spin disorder, facilitate an additional interparticle interaction mechanism: superexchange. We attribute an observed hardening of the magnetic field response at low temperature and the appearance of a superspin glass transition to the onset of interparticle superexchange along the assembly series.

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