

#ESMoINa

2024

**17th European School
on Molecular Nanoscience**
(ESMoINa2024) **19th - 24th May 2024**

10th Workshop on 2D Materials
(W2DM2024) **23rd and 24th May 2024**

#esmolna2024

Cuenca. (Spain)



Organized by:



Sponsors:



**Nano
Mol
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W
2d_m
Workshop on
2D Materials

May 2024	Sunday 19 th	Monday 20 th	Tuesday 21 st	Wednesday 22 nd	Thursday 23 rd	Friday 24 th	May 2024
9:00-9:30		A. Ardavan	G. Chastanet	L. Bogani	N. Pascual		9:00-9:30
9:30-10:00		Y. Manassen	J. Rodríguez	J. Soriano	M. Moreno	Brainstorming session:	9:30-10:00
10:00-10:30		S. Chorazy	M. Souto	G. Aromí	E. Vázquez		10:00-10:30
10:30-11:00		Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	10:30-11:00
11:00-11:30							11:00-11:30
11:30-12:00		D. Écija	C. Romero	A. Lunghi	E. Cánovas	Trends & perspectives in 2D Materials	11:30-12:00
12:00-12:30		P. Marín	S. Wuttke	H. Suderow	A. Forment		12:00-12:30
12:30-13:00			R. Torres		C. Boix		12:30-13:00
13:00-13:30						LUNCH	13:00-13:30
13:30-14:00		LUNCH	LUNCH	LUNCH	LUNCH		13:30-14:00
14:00-14:30							14:00-14:30
14:30-15:00							14:30-15:00
15:00-15:30							15:00-15:30
15:30-16:00							15:30-16:00
16:00-16:30	Registration						16:00-16:30
16:30-17:00	Welcome	M.J. Martínez	M. Varela	S. Carretta	J. Lado		16:30-17:00
17:00-17:30		Oral Comm.	Oral Comm.	Oral Comm.	M. Morant		17:00-17:30
17:30-18:00		Coffee break	Coffee break	Coffee break	Coffee break		17:30-18:00
18:00-18:30	F. Zamora	Oral communications & Flash presentations	Oral communications & Flash presentations	Oral communications & Flash presentations	Oral comm. & Flash presentations		18:00-18:30
18:30-19:00	R. Sanchis						18:30-19:00
19:00-19:30	Reception cocktail				Closing & awards		19:00-19:30
19:30-20:00							19:30-20:00
20:00-20:30							20:00-20:30
20:30	DINNER	DINNER	DINNER	DINNER	COCKTAIL DINNER		20:30

Molecular Nanoscience

The molecular region of Nanoscience is still a region that has been scarcely explored in Nanoscience, maybe because the larger structural and electronic complexity of molecules, compared with that found in simpler atom-based nano-objects and nanostructures, make them more difficult to study at the nanoscale with the currently available instrumental techniques. Albeit, it is in this molecular region where molecular chemists, biologists, physicists and engineers working in Nanoscience may find the best opportunities to interact and to converge. Areas like supramolecular chemistry, molecular electronics and molecular magnetism are expected to converge in this region.

The School

The 17th European School on Molecular Nanoscience (ESMoINa2024) 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.

The Workshop on 2D Materials

The 10th Workshop on 2D Materials (W2DM2024) will take place on May 23rd and 24th 2024, having the first day a joint program with ESMoINa2024.

Graphene and other two-dimensional (2D) materials represent one of the priority areas of the European Commission, as shown by the 'Graphene flagship'. Due to the exceptional mechanical and electronic properties of graphene, research about this material has been at the forefront of this area during the last years. However, other 2D materials, like metal chalcogenides or molecular-based layers are emerging. In these materials a wide range of properties can be found, including superconductivity and magnetism. The research community exploring graphene and other 2D materials is increasing, due to the incorporation of researchers from a variety of fields like materials science, physics, chemistry and engineering. Moreover, there is a big interest in the construction of functional heterostructures and devices based on 2D materials, including their integration with graphene.

During the W2DM2024 collaboration among participant researchers will be promoted, in order to face the huge scientific challenges encountered in this field, both from an experimental and theoretical point of view.

Organizers & Committee

Organizers

These school are organized by the Institute of Molecular Science (ICMol) of the Universitat de València and the Faculty of Environmental Sciences and Biochemistry of the Universidad de Castilla- La Mancha.

Committee



Eugenio Coronado

Chair

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



Fernando Langa

Chair

Universidad de Castilla - La Mancha
Spain

Conference Secretary:

Paco Escrig Escrig

francisco.escrig@uv.es

Institut de Ciència Molecular. Universitat de València

Invited Speakers



Arzhang ARDAVAN

U. Oxford (UK)



Lapo BOGANI

U. Firenze (IT) & U.
Oxford (UK)



Stefano CARRETTA

U. Parma (IT)



Guillaume CHASTANET

I. Condensed Matter
Chemistry of Bordeaux
(ICMCB)-CNRS (FR)



David ÉCIJA

IMDEA Nanoscience (ES)



José LADO

U. Aalto (FI)



**M^a José MARTÍNEZ
PÉREZ**

I. Nanoscience and
Materials of Aragon
(INMA)-CSIC- U.
Zaragoza (ES)



Nacho PASCUAL

CIC NanoGUNE (ES)



María VARELA

U. Complutense Madrid
(ES)



Felix ZAMORA

U. Autónoma Madrid (ES)

**More
information
about the
speakers**



www.icmol.es/esmolna2024/

Structure & Topics

The School is structured in three different blocks:

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.



The electronic version of lectures and seminars can be found on the School electronic book: <http://www.icmol.es/esmolna2024/ebook.php>



Location / Cuenca

The 17th European School on Molecular Nanoscience (ESMoI Na2024) and the 10th Workshop on 2D Materials (W2DM2024) will take place in Cuenca. The town of Cuenca is located in the interior of Spain, in the northeast of the Castile-La Mancha region.

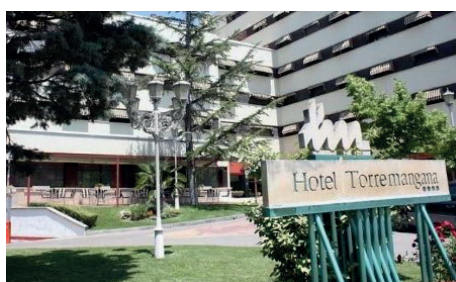
The most outstanding feature of the city is its beauty that arises, on the one hand, from the harmony between nature and architectural space and, on the other hand, from its long historical trajectory that has left us an important cultural and monumental legacy.

On 1996 Cuenca was named a World Heritage Site by UNESCO thanks to the excellent preservation of its original urban landscape, medieval fortress and its rich collection of civil and religious architecture from the twelfth to the eighteenth centuries. In addition, the city has an exceptional personality as it is perfectly integrated into the wonderful natural landscape that surrounds it.



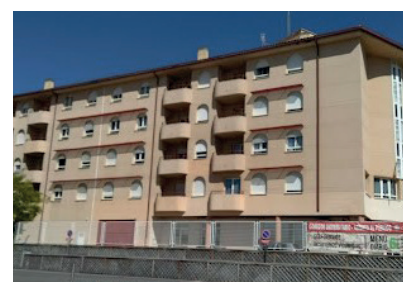
Talks

Gil Albornoz Building
Social Sciences Faculty
(ULCM). Conference Hall (Salón
de actos)
Av. de los Alfares, 44



Accommodation & dinner

Hotel Torremangana
Av. San Ignacio
de Loyola, 9



Lunch

**Juan Giménez de
Aguilar cafeteria**
Camino Nohales, s/n



08h00 SUNDAY 19th - ESMoLNa		
16h00	Registration	
17h00	Eugenio CORONADO- ICMol- U. València (ES) & Fernando LANGA- U. Castilla- La Mancha (ES)	<i>Welcome & Introduction to Molecular Nanoscience</i>
18h00	Félix ZAMORA- U. Autónoma Madrid (ES)	<i>Exploring Design and Processability of Imine-Based Covalent Organic Frameworks (COFs)</i>
19h00	Roger SANCHIS GUAL- ICMol- U. València (ES)	<i>Multifunctional microrobots for biomedical applications</i>
19h30	<i>Reception cocktail</i>	
20h30	<i>Dinner</i>	
08h00 MONDAY 20th - ESMoLNa		
09h00	Arzhang ARDAVAN- U. Oxford (UK)	<i>Some ingredients for practical molecular quantum technologies</i>
10h00	Yishay MANASSEN- Ben Gurion U. (IL)	<i>STM NMR of single atom and single molecule - simple and complicated molecules</i>
10h30	Szymon CHORAZY- Jagiellonian U. (PL)	<i>Optical Thermometers Based on Single-Molecule Magnets - A Heterometallic Approach</i>
11h00	<i>Coffee break</i>	
11h30	David ÉCIJA- IMDEA Nanoscience (ES)	<i>On-surface synthesis</i>
12h30	Pilar MARÍN PALACIOS- Applied Magnetism Inst. (IMA) (ES)	<i>New Trends on Magnetic Sensors</i>
13h30	<i>Lunch</i>	
16h30	M^a José MARTÍNEZ PÉREZ- INMA-CSIC- U. Zaragoza (ES)	<i>Spin-spin interactions in cavity quantum electrodynamics</i>
17h30	ARROYO - FRUCTUOSO Alba- ICMol- U. València (ES)	<i>Advanced 3D nano-object patterning for AFM topographic measurements</i>
17h40	GÓMEZ MUÑOZ Iván- ICMol- U. València (ES)	<i>A Dynamic Lanthanide-Organic Framework: Flexibility and Implementation of Magnetic Properties on Demand</i>
17h50	EL ALOUANI DAHMOUNI Nadia- ICMol- U. València (ES)	<i>Atypical Magnetic Field Effects on the Slow Magnetic Relaxation and Magnetocaloric Efficiency of a Tetranuclear Neodymium(III)-Nickel(II) Complex</i>
18h00	<i>Coffee break</i>	
18h30	GIMENEZ- SANTAMARINA Silvia- ICMol- U. València (ES)	<i>Electronic structure calculations of Fe(II) SCO complexes: accuracy of post-Hartree Fock methods</i>
18h40	DZIERŻEK Dominik- Jagiellonian U. (PL)	<i>Metal complexes of a new tris(dioxothiadiazole) ligand - towards magnetic and electro-chemically active coordination frameworks</i>
18h50	GŁOSZ Dorota- Jagiellonian U. (PL)	<i>Anion-π bonds stabilize the elusive C6O6 oxocarbon</i>
19h00	WOTA Gaja- Jagiellonian U. (PL)	<i>Dehydration-driven metal-to-metal charge transfer in a Ni-Ru CN-bridged chain</i>
19h10	LEVY Gilad- The Weizmann Inst. of Science (IL)	<i>Peltier cooling in an atomic scale all-metal Kondo system.</i>
19h20	DELGADO GARCÍA Rafael- U. Castilla - La Mancha (ES)	<i>Magnetometry study of a 3D corrugated magnetic thin film with antiparallel domain configuration</i>
19h30	MCLARNON Bob- ICMM - CSIC (ES)	<i>Low-Cost Nano Lithography using Commercial 3D UV Resin printers.</i>
19h35	ORDIALES CABALLERO Carolina- IMDEA Nanoscience / UAM (ES)	<i>Tuning PDMS surface properties for Organ-on-chip devices applications</i>
19h40	LARGO BARRIENTOS Antonio- U. Valladolid (ES)	<i>Influence of infrared blocker content on the thermal conductivity of microcellular PMMA.</i>
20h30	<i>Dinner</i>	

08h00 TUESDAY 21st - ESMoLNa		
09h00	Guillaume CHASTANET- I. Condensed Matter Chemistry of Bordeaux (ICMCB)-CNRS (FR)	Spin Crossover Particles: Exploring New Processes for the Synthesis of Nanoparticles and Nanocomposites
10h00	Jorge RODRÍGUEZ NAVARRO- U. Granada (ES)	<i>Metal-organic assemblies for detoxification of harmful molecules</i>
10h30	Manuel SOUTO SALOM- CiQUS- U. Santiago Compostela (ES)	<i>Redox-active Covalent Organic Frameworks as promising organic electrodes for metal-ion batteries</i>
11h00	<i>Coffee break</i>	
11h30	Carlos ROMERO NIETO- U. Castilla-La Mancha (ES)	<i>What can phosphorus heterocycles provide to materials science?</i>
12h00	Stephan WUTTKE- BCMaterials (ES)	<i>Reticular Nanoscience: Bottom-Up Assembly Nanotechnology</i>
12h30	Ramón TORRES CAVANILLAS- Oxford U. (UK)	<i>Synthesis of 2D Materials Beyond Graphene for Next-Generation Stimuli-Responsive Devices</i>
13h30	<i>Lunch</i>	
16h30	María VARELA- U. Complutense Madrid (ES)	Atomic resolution in-situ studies of nanomaterials
17h30	Clara CHINCHILLA GARZÓN- ICMol- U. València (ES)	<i>Isorecticular Expansion and Linker-Enabled Control of Interpenetration in Titanium–Organic Frameworks</i>
17h40	Jaime GARCÍA CABA- ICMol- U. València (ES)	<i>Biocompatible Zn metal-organic framework for drug capture</i>
17h50	Lidia GARCÍA LOPEZ- ICMol- U. València (ES)	<i>Design of novel Metal Organic Frameworks built from oxamate functionalized amino acid ligands</i>
18h00	<i>Coffee break</i>	
18h30	Jesús Antonio CASES DÍAZ- ICMol- U. València (ES)	<i>Boosting protein encapsulation through Lewis-acid-mediated MOF mineralization: toward effective intracellular delivery</i>
18h40	Luis LEÓN ALCAIDE- ICMol- U. València (ES)	<i>Solvent-Free Synthesis for Harvesting Novel Melting MOFs</i>
18h50	Thibaut LE HUEC- ICMol- U. València (ES)	<i>MOF-on-MOF heterostructures for water splitting photocatalysis under solar light</i>
19h00	Beatriz MEANA BAAMONDE- ICMol- U. València (ES)	<i>Photo-organocatalytic decarboxylative borylation</i>
19h05	Eloy Pablo GÓMEZ DE OLIVEIRA- ICMol- U. València (ES)	<i>Integrating Compositional and Structural Framework Diversity by Metal-Exchange Methods</i>
19h10	María TAMAYO FRAILE- ICMol- U. València (ES)	<i>Ultrastable Pyrazolate Porphyrin Metal-Organic Frameworks for environmentally relevant applications</i>
19h15	Maria Amparo LOPO MARCH- ICMol- U. València (ES)	<i>Development of multifunctional architectures to target G4s and deliver anticancer drugs.</i>
19h20	Leyre Bei FRAILE AGUIRRE- U. Autónoma Madrid (ES)	<i>A radiofrequency study of nanoparticles deposited on solids for sensing applications</i>
19h25	Ángela FERNÁNDEZ COBO- U. Autónoma Madrid (ES)	<i>Mesoporous nanocatalysts based on Pd for bioorthogonal chemistry</i>
19h30	Carmen VICIANA- U. Autónoma Madrid (ES)	<i>Harnessing Metal-Organic Frameworks for multi-contaminant water treatment</i>
19h35	Jialei CHEN QIU- U. Autónoma Madrid (ES)	<i>Post-functionalization of Covalent Organic Frameworks aerogels</i>
19h40	Johana HERRERO ACEITUNO- U. Autónoma Madrid (ES)	<i>Removal of pharmaceutical pollutants by hydrogels of Covalent Organic Frameworks.</i>
19h45	Ángel María PRIOR PERAL- U. Miguel Hernández (ES)	<i>Synthesis of a perylenediimide-galactose-phenanthroline conjugate for cancer therapy</i>
19h50	Pablo RODRIGUEZ ALONSO- U. Valladolid / TPNBT SL (ES)	<i>Elastin-like recombinamers hydrogels: thermosensitivity and cellular response</i>
20h30	<i>Dinner</i>	

08h00 WEDNESDAY 22nd- ESMoINa		
09h00	Lapo BOGANI- U. Firenze (IT)	The fourth Carbon wave: organic and inorganic molecular chemistry for quantum devices
10h00	Joaquín SORIANO LÓPEZ- ICMol- U. València (ES)	<i>Water Oxidation Electrocatalysis Promoted by Hybrid Polyoxometalate/Layered Double Hydroxide Nanocomposites</i>
10h30	Guillem AROMÍ- U. Barcelona (ES)	<i>Magnetism and photophysics of heterometallic lanthanide coordination complexes</i>
11h00	<i>Coffee break</i>	
11h30	Alessandro LUNGI- Trinity College Dublin (IE)	<i>Relaxation and decoherence in magnetic molecules</i>
12h00	Hermann SUDEROW- U. Autónoma Madrid	Superconductivity and electronic correlations in two dimensions
13h30	<i>Lunch</i>	
16h30	Stefano CARRETTA- U. Parma (IT)	Molecular nanomagnets: a viable path toward quantum information processing?
17h30	Joseline IRIBARRA ARAYA- ICMAB-CSIC (ES)	<i>New styryldiazepinoporphyrazines from CCMoids for coordination polymers</i>
17h40	Pablo NAVARRO MADRAMANY- ICMol- U. València (ES)	<i>Nanozymes Mimicking Superoxide Dismutase: An Outstanding Antioxidant Performance</i>
17h50	Abin GEORGE- U. Valladolid (ES)	<i>Voltammetric MIP (Molecularly imprinted polymer) sensor for sugar detection using nanoparticle and chitosan</i>
17h55	Antonio Joaquin MARTIN PINILLOS- U. Valladolid (ES)	<i>Enhancing chitosan-based MIPs capabilities for wine compounds.</i>
18h00	<i>Coffee break</i>	
18h30	Sebastian VAN DER POEL- Delft U. Technology (NL)	<i>A Mechanosensitive Naphtalenophane as Platform for Quantum Interference Studies</i>
18h40	Dawid KRUCZEK- Jagiellonian U. (PL)	<i>Ce(III)-Pt(II) based coordination networks as magnetic luminophores sensitive to solvent vapors</i>
18h50	Katarzyna RZEPKA- Jagiellonian U. (PL)	<i>Optically pure propeller-shaped lanthanide single molecule magnets with helicene ligands</i>
19h00	Kinga SZCZECIŃSKA- Jagiellonian U. (PL)	<i>Dielectric relaxations and photoluminescent properties in ionic salts based on the dicyanido-bis(2,2'-phenylpyridinate)rhodate(III) anion.</i>
19h10	Marta NIEMIEC- Jagiellonian U. (PL)	<i>Heterometallic s-d frameworks with hexacyanidometallates for the construction of luminescent sensors</i>
19h20	Mar FERRI CORTÉS- U. Alacant (ES)	<i>Quantum computation in atomic and molecular lattices</i>
19h30	Tamara DONATE RIVAS- ICMol- U. València (ES)	<i>Sublimed Texture Tandem Silicon/Perovskite Solar Cells</i>
19h35	Ana PUCHADES ORTIZ- ICMol- U. València (ES)	<i>Stability of HTLs in co-evaporated perovskite solar cells with substrate configuration</i>
19h40	Adriana AGRAMUNT- U. Autónoma Madrid (ES)	<i>Novel donor-acceptor dyads based on 30-pi electron expanded hemiporphyrines</i>
19h45	Lucia PALOMINO RUIZ- U. Granada (ES)	<i>Defective nanographenes: synthesis and electron-transport properties at the single-molecule scale</i>
19h50	Jesús Gabriel MADRID NEGRÍN- U. La Laguna (ES)	<i>La_{2-x}CaxSc_{1-y}MgyNbO_{7-δ}: Proton-conducting Ceramic Materials for Proton Ceramic Fuel Cells</i>
19h55	Ilenia PASCALE- U. Castilla - La Mancha (ES)	<i>Chemical modification of 7,6-SWCNTs by Pd-porphyrin derivatives through different covalent approach</i>
20h30	<i>Dinner</i>	

THURSDAY 23rd - ESMoLNa & W2DM		
09h00	Natxo PASCUAL- CIC NanoGUNE (ES)	<i>Inducing magnetism and superconductivity in graphene</i>
10h00	Miguel MORENO UGEDA- Donostia International Physics Center (DIPC) (ES)	<i>Unveiling the nature of superconductivity in octahedrally coordinated (1T) layered dichalcogenides</i>
10h30	Ester VÁZQUEZ PACHECO- IRICA- U. Castilla- La Mancha (ES)	<i>Challenges in the biological application of 2D materials: toxicological testing</i>
11h00	<i>Coffee break</i>	
11h30	Enrique CÁNOVAS- IMDEA Nanoscience/Max Planck for Polymer Research (ES/DE)	<i>Non-contact electrical characterization of 2D MOFs and COFs by time resolved THz spectroscopy</i>
12h00	Alicia FORMENT ALIAGA- ICMol- U. València (ES)	<i>AFM as a tool for 2D materials</i>
12h30	Carla BOIX CONSTANT- ICMol- U. València (ES)	<i>Strain Switching in van der Waals Heterostructures Triggered by a Spin-Crossover Metal–Organic Framework</i>
13h30	<i>Lunch</i>	
16h30	José LADO- U. Aalto (FI)	<i>Engineering artificial quantum matter with two-dimensional materials</i>
17h30	Marc MORANT GINER- ICMol- U. València (ES)	<i>MoS2 for different applications: from biomedicine to catalysis</i>
18h00	<i>Coffee break</i>	
18h30	Yousra DIOUANE- ICMol- U. València (ES)	<i>Impact of Pseudohalide Substitution on the Electrochemical and Magnetic Behavior of α Cobalt-Based Layered Hydroxide Materials</i>
18h40	Andrey RYBAKOV- ICMol- U. València (ES)	<i>Twisted magnetic multilayers of CrSBr</i>
18h50	Rebeca MARTINEZ HAYA- ICMol- U. València (ES)	<i>Exploring the interaction and reactivity in graphene-antimonene heterostructures</i>
19h00	Marc LÓPEZ MOLLA- ICMol- U. València (ES)	<i>Synthesis of graphene-layer double hydroxide hybrids for catalytic applications.</i>
19h05	Ricardo AGUADO COLLAZO- ICMol- U. València (ES)	<i>Magnetoelectric effect on Van der Waals heterostructures</i>
19h10	Turlough BRENNAN- ICMol- U. València (ES)	<i>Hyperspectral Microscopy for the study of layer dependent optical properties of different two-dimensional materials.</i>
19h15	Álvaro CORTÉS FLORES- U. Alicante (ES)	<i>Biaxial Strain of Single-Layer WS₂ Over a Wide Range of Temperature</i>
19h20	Susana ABERTURAS LÓPEZ- U. Autónoma Madrid (ES)	<i>Growth and characterization of Ni-Fe ultra-thin films on different buffer layers</i>
19h25	Simeon NIKOLAEV VLADIMIROV- U. Autónoma Madrid (ES)	<i>Improved strain engineering of atomically thin MoS2 by polymer encapsulation</i>
19h30	Closing and GENAM-RSEQ Awards to the best Flash Presentation or Oral Communication	
20h30	<i>Cocktail Dinner and music</i>	
FRIDAY 24th - W2DM		
09h30	Brainstorming session: Trends and perspectives in 2D Materials	
11h00	<i>Coffee break</i>	
11h30	Brainstorming session: Trends and perspectives in 2D Materials	
13h00	<i>Finger Lunch</i>	

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Advanced 3D nano-object patterning for AFM topographic measurements

Alba ARROYO-FRUCTUOSO¹, Ana GALET¹, Gregor HLAWACEK², and Rosa CÓRDOBA¹.

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Atomic Force Microscope (AFM) is a technique that enables the measurement of topography of a sample surface achieving a high nanometric resolution. Presently, there is a notable emphasis on the fabrication of advanced probes through 3D nanoprinting methods due to the advancements in the realization of measurements such as electrical, thermal, magnetic, surface strength, and biological^[1] properties. In particular, the utilization of focused ion beam induced deposition (FIBID) technique is capable of partially decomposing precursor molecules to generate nano-deposits in a single step^[2]. To date, the published works on FIBID technique have predominantly centred around a single geometry: nanopillars^[3,4].

In this study, we utilized He⁺ FIBID as a 3D nanoprinting technique to fabricate advanced 3D W-C nano-objects in a direct step onto commercial AFM probes. The characteristics of the probes are defined by curvature radius, half-cone angle and the probe length. To study these characteristics, three different geometries have been fabricated: nanohelices, nanopillars, and nanospirals. The dimensions of each probe have been varied and studies of topography and surface roughness have been carried out. The fabricated advanced probes were utilized in two set of AFM measurements and they were inspected in a Scanning Electron Microscope before being reused. The results of the second set of measurements closely resembled those of the first, indicating the robustness of the probes. Additionally, they demonstrate durability and resilience over time, as evidenced by their capability to measure surfaces effectively two years after fabrication.

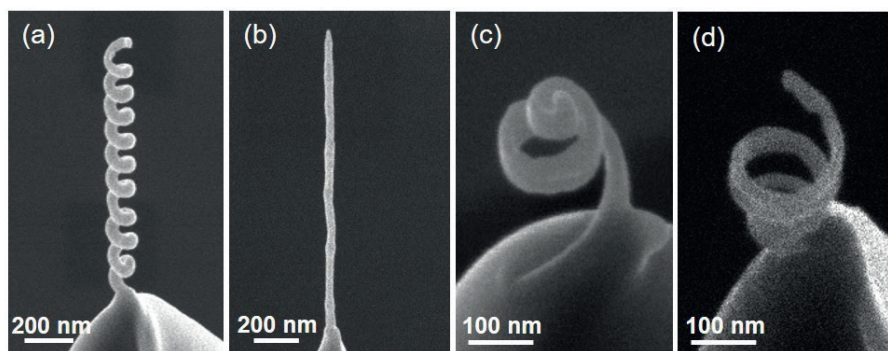


Figure 1: HIM images illustrate advanced probes exhibiting diverse 3D geometries fabricated by He⁺ FIBID: (a) R-nanohelix, (b) Nanopillar, (c) Inward Archimedean nanospiral, and (d) Outward Archimedean nanospiral.

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A Dynamic Lanthanide-Organic Framework: Flexibility and Implementation of Magnetic Properties on Demand

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In this work we report the synthesis of a lanthanide-organic framework (LOF)^[1] with a dynamic structure that provides electable magnetic properties. Breathing and gate-opening phenomena are triggered by the variation of the DMF content and N₂ sorption, resulting in the formation of new crystal phases with different properties. The originally diamagnetic structure can be provided with magnetic properties by the incorporation of small amounts of paramagnetic elements from the lanthanide series (*ie.* Dy or Gd) during the synthesis. While the desolvated form exhibits an excellent performance as a Single-Ion Magnet (SIM)^[2], the fully activated structure presents outstanding qubit properties^[3]. Moreover, the responsive behavior of the compound was also confirmed to have an impact on the qubit properties upon the adsorption of N₂. The noticeable differences in the spectra of the sample in the presence and absence of N₂ highlight the potential application of the material as a sensor to detect this gas even at room temperature.

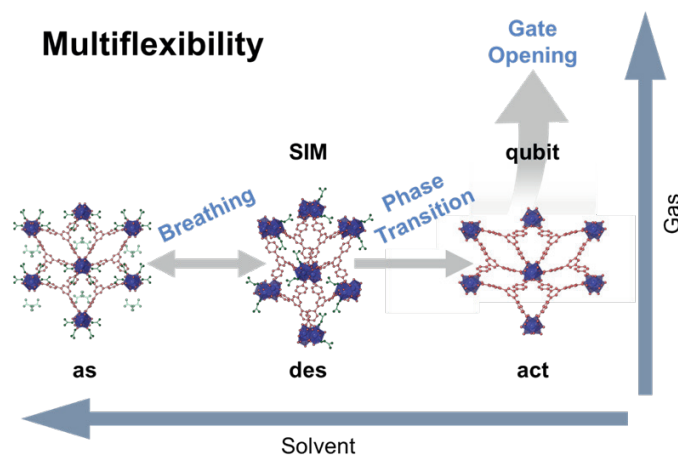


Figure 1. The framework undergoes different phase transitions with unique properties.

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Atypical Magnetic Field Effects on the Slow Magnetic Relaxation and Magnetocaloric Efficiency of a Tetranuclear Neodymium(III)-Nickel(II) Complex

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Mixed 4f/nd (n = 3–5) polynuclear complexes, referred to as metal-organic clusters (MOCs), offer unique examples of single-molecule magnets (SMMs) for nanotechnological applications in cryogenic magnetic refrigeration (CMR) [1].

A field-induced blockage of the magnetization occurs in the starlike heterotetranuclear complex of formula $(\text{Me}_4\text{N})_3\{\text{Nd}(\text{H}_2\text{O})_3[\text{Ni}(\text{dto})_2]_3\} \cdot \text{H}_2\text{O}$ (**1**) prepared from the use of the diamagnetic bis(dithiooxalato)nickel(II) complex as metalloligand toward the magnetically anisotropic fully solvated neodymium(III) ion. The inverse field dependence of the spin dynamics featuring a low-field slower-relaxing (SR) and a high-field faster-relaxing (FR) Nd^{III} ions, combined with significant magnetocaloric effects at low temperatures and magnetic field changes, make **1** a suitable candidate as magnetic field-effect spin quantum transistor and molecular cryomagnetic cooler, enlarging thus the variety of applications of this simple class of multiresponsive and multifunctional 4f/3d-mixed molecular nanomagnets.

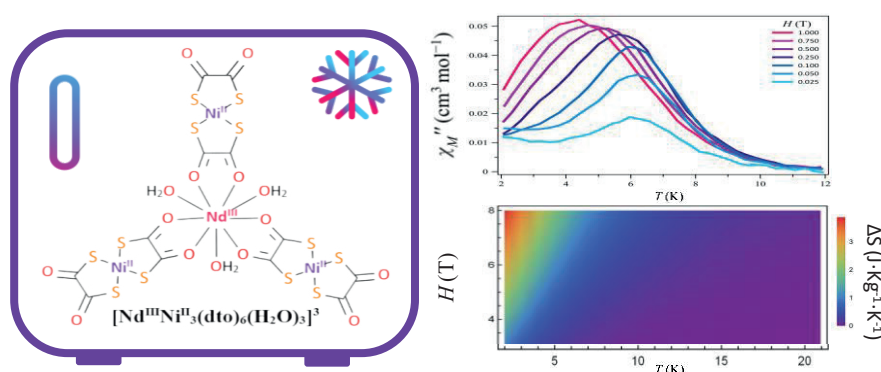


Figure 1.

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Electronic structure calculations of Fe(II) SCO complexes: accuracy of post-Hartree Fock methods

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From the theoretical point of view, the modelling of Spin Crossover (SCO) compounds presents important challenges due to the complexity of all the interactions involved in the compounds showing externally activated spin transitions.

In this project we intend to deepen in the very well-known problem regarding the accurate description of the electronic configuration of SCO compounds. We used as a benchmark a series of SCO based on Fe(II) of different sizes and simulated their electronic structures in High and Low Spin states (HS, LS). We have compared systematically the accuracy of different post-Hartree-Fock Quantum Mechanics models, ranging from Configuration Interaction (CI), Complete Active Space Self-Consistent Field (CASSCF), N-electron Valence and Multireference Perturbation theory (NEV/CASPT2) at predicting the energy splitting between HS and LS. Our results are compared with values obtained by diffusion Monte Carlo (DMC) taken as reference [1].

We have seen that NEVPT2 energies are comparable to CCSD(T), while CASPT2 are in the range of DMC method. By comparing Active Space sizes, we detected that NEVPT2 methods shows a higher dependence. By means of Difference Dedicated Configuration Interaction (DDCI) method, we reached the best accuracy to the chosen reference values. We will briefly discuss the intrinsic limitations across methodologies and discuss the dependence of the ordering in energy of the different spin states [2].

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Metal complexes of a new tris(dioxothiadiazole) ligand - towards magnetic and electro-chemically active coordination frameworks

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In the search for a new group of versatile organic building blocks, potentially useful in the design of switchable molecular magnetic materials, dioxothiadiazoles (1,2,5-thiadiazole 1,1-dioxides) were proposed as promising candidates [1]. The tripak moiety, recently reported by Pakulski *et al.* [2], is of particular interest due to its rich electrochemistry and ability to form persistent radicals that can prove advantageous for potential applications in magnetism and molecular electronics.

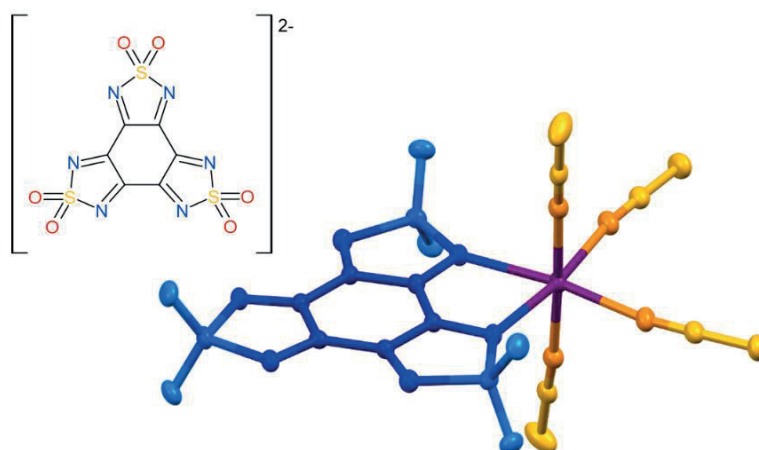


Figure 1. Structure of $[M^{II}(\text{CH}_3\text{CN})_4][\text{tripak}]$ molecule along with a structural formula of the tripak dianion ($M = \text{Cr}, \text{Mn}, \text{Fe}, \text{Cu}, \text{Zn}$)

The bis(thiadiazole) backbone makes tripak a potential trischelating N,N-donor ligand for the design of metal-organic coordination frameworks. Designing a compound containing both d-block metal cations and tripak anions is highly desirable due to the potential interactions between these building blocks. In pursuit of this goal, a series of compounds with a general formula $[M^{II}(\text{CH}_3\text{CN})_4][\text{tripak}]$ where $M^{II} = \text{Cr}, \text{Mn}, \text{Fe}, \text{Cu},$ and Zn has been prepared and characterised by sc-XRD, PXRD, CV and SQUID magnetometry. Currently, efforts are being made to implement various oxidation states of tripak and explore charge transfer mechanisms.

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Anion- π bonds stabilize the elusive C_6O_6 oxocarbon

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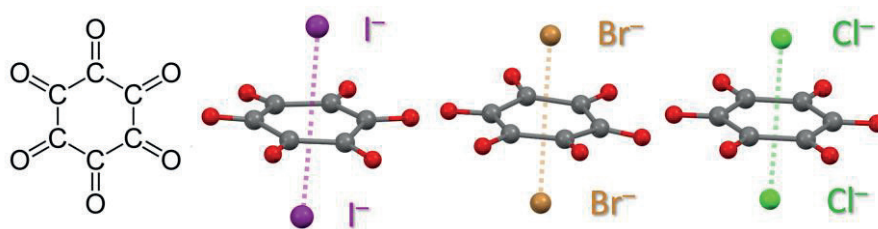
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Cyclohexanehexone (also known as hexaketocyclohexane) C_6O_6 or $(CO)_6$ is a fascinating and yet an unknown oligomer of carbon monoxide. Its elusive character is due to the lack of thermodynamic stability.^[1] Its fully hydrated form – dodecahydroxycyclohexane ($C_6O_{12}H_{12}$) – is commercially available but it does not bear any electronic features of the original with all carbons being sp^3 . The dianionic congener – the well-known rhodizonate anion $C_6O_6^{2-}$ – is aromatic^[1] and widely used in coordination chemistry and crystal engineering.^[2] C_6O_6 , on the other hand, despite being flat, is non-aromatic and has a completely empty π orbital. Computational studies suggest that it would have the potential to form the strongest anion- π interactions if it could be isolated.^[3]

Herein, we present a series of three anion- π reverse-sandwich complexes of C_6O_6 with halide anions: $C_6O_6@2Cl^-$, $C_6O_6@2Br^-$ and $C_6O_6@2I^-$ accompanied by two bulky organic counterions. The single crystal X-ray diffraction structural analysis of these supramolecular complexes reveal the shortest ever reported distances between the centroid of the C_6O_6 ring and the halide anions: 2.359 Å, 2.549 Å and 2.754 Å for Cl^- , Br^- , and I^- , respectively (see Figure below). Summarizing, the formation of sandwich anion- π complexes enabled observation and unequivocal identification of the C_6O_6 molecule for the first time. The complexes are stable in MeCN solution and the halides can be exchanged between each other in the following sequence: I^- to Br^- to Cl^- . This has been demonstrated by ^{13}C NMR as well as infrared spectroscopy.



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Dehydration-driven metal-to-metal charge transfer in a Ni-Ru CN-bridged chain

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Materials which show response to external stimuli like temperature, pressure or humidity are widely studied as potential chemical sensors. Beside the changes of other measurable properties e. g. proton/electron conductivity or magnetic behaviour, the visible difference in colour is regarded a desired factor in molecular indicators, since it makes them easy to use, without any electronic equipment. The $\{\text{NH}_4[\text{Ni}(\text{cyclam})][\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}\}_n$ chain [1] is an interesting example of a multi-switchable non-rigid cyano-bridged coordination system. It shows metal-to-metal charge transfer (MMCT) which can be controlled by temperature, pressure, and humidity. At ambient conditions it can coexist in three phases differing in colour and magnetic properties: red HT, blue LT, and greenish-yellow dehydrated phase.

To explore the possibility of tuning the MMCT process characteristics we replaced iron(II) with ruthenium(II), which is known to show similar behaviour in related coordination system [2]. As a result of the reaction between $[\text{Ni}(\text{cyclam})]^{3+}$ and $[\text{Ru}(\text{CN})_6]^{4-}$ ions in concentrated NH_4Cl solution, we isolated two coordination polymers: the analogue of the 1D Ni-Fe structure $\{\text{NH}_4[\text{Ni}(\text{cyclam})][\text{Ru}(\text{CN})_6] \cdot 5\text{H}_2\text{O}\}_n$ (**1**), which is formed after one week, and the 2D honeycomb-like network (**2**), which precipitates initially. Both compounds undergo MMCT process from $\text{Ni}^{\text{III}}\text{-Ru}^{\text{II}}$ to $\text{Ni}^{\text{II}}\text{-Ru}^{\text{III}}$ upon dehydration, which results in changes of colour and magnetic susceptibility. The magnetic measurements for **1** indicate that the electron transfer occurs in 50% of metal centres. The PXRD and spectroscopic studies show that the rehydration process is only partly reversible.

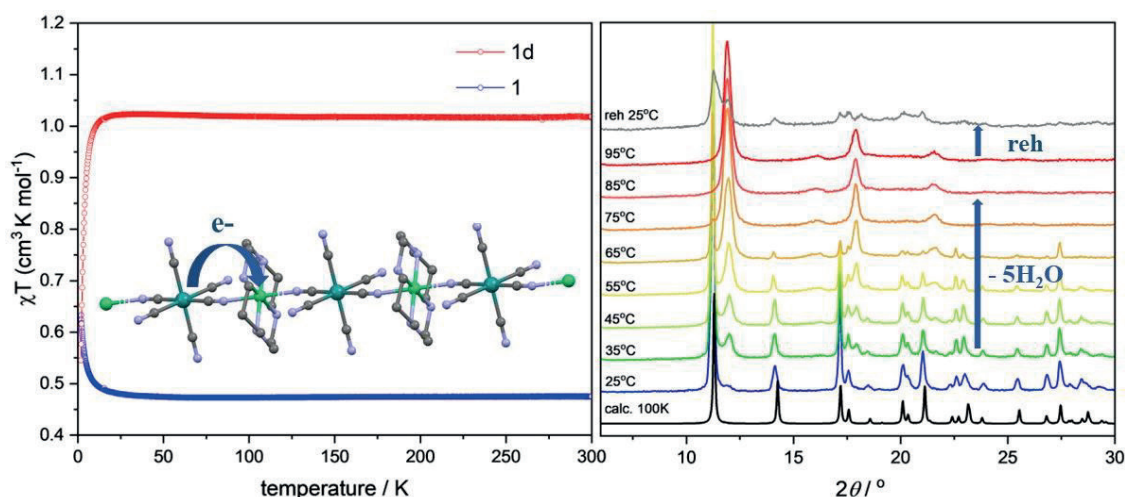


Figure. Structure of **1** and its magnetic susceptibility in the hydrated (**1**) and dehydrated (**1d**) form (left); thermal dehydration and rehydration process followed by PXRD (right).

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Peltier cooling in an atomic scale all-metal Kondo system

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At the nano-scale, heat dissipation emerges as a critical challenge in the design of electronic devices. Yet, quantum phenomena can open the door for nano-scale heat pump realizations for efficient thermal management. In this work, we demonstrate for the first time an all-metal atomic-scale heat pump. Specifically, we have embedded a microscale thermometer 400 nm away from an atomic-scale break junction. The junction is made of an Au neck of several atoms in diameter, doped with Cr. In this system, Kondo transport in combination with quantum interference yields significant Peltier cooling with a Seebeck coefficient higher by two orders of magnitude than found for any other metallic system. We thus demonstrate a unique atomic scale system that can serve as a testbed for the study of quantum thermodynamics, with heat pumping that is significant enough for future applications in the form of arrays of such junctions. Furthermore, the fabricated device and the ability to measure temperature at the nanoscale vicinity of a junction lay the foundations for a follow up study of heat dissipation in molecular junctions using the same setup.

Magnetometry Study of a 3D Corrugated Magnetic Thin Film with Antiparallel Domain Configuration

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Three-dimensional magnetic structures have direct applications in magnetic field sensing [1] or non-conventional computing [2]. New nanostructuring procedures allow the fabrication of well-defined nano-undulated ferromagnetic thin films. The structural modulation can form appealing 3D magnetic patterns during magnetization reversal as demonstrated in references [3] and [4]. However, the study of the magnetic reversal properties of such systems presents many challenges due to the low dimension of the magnetic features and their interplay with optical phenomena. We present an experimental study on the magneto-optical response of a 3D corrugated ferromagnetic thin film fabricated with a combination of laser interference lithography and DC sputtering techniques (Fig.1 a) [4]. We perform angular Kerr measurements with different light colours such that the pattern features fall either in the subwavelength (red light) or in the diffraction regime (violet light). Violet Kerr measurements show new features on the magnetization reversal (Fig.1 b) that we associate to the formation of 3D antiparallel magnetic domains. We confirm this magnetic distribution with micromagnetic simulations (Fig.1 c) and magnetic force microscopy measurements at remanence. The occurrence of 3D magnetic states and the magneto-optical features associated with the diffraction regime characteristics in the studied system make it a promising material for magnetic sensing or computing applications.

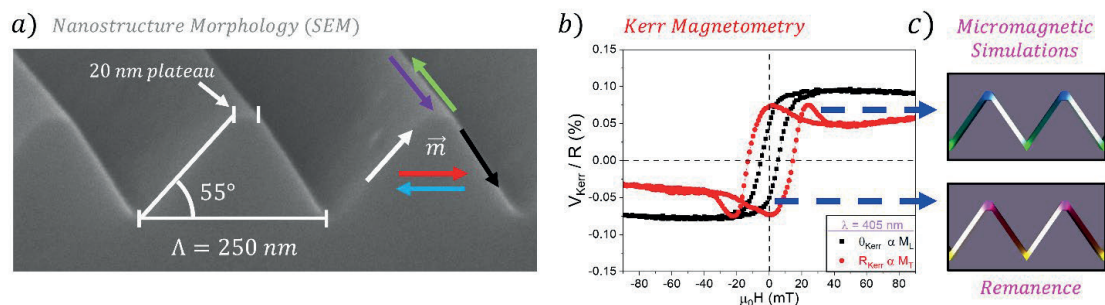


Figure 1. a) Nanostructure morphology of the corrugated sample obtained with lateral SEM, color scheme for micromagnetic simulations is shown in arrows, b) Violet Kerr effect measurements of Py-ST sample on hard axis, c) Micromagnetic simulations of relevant magnetic states during the magnetization reversal process.

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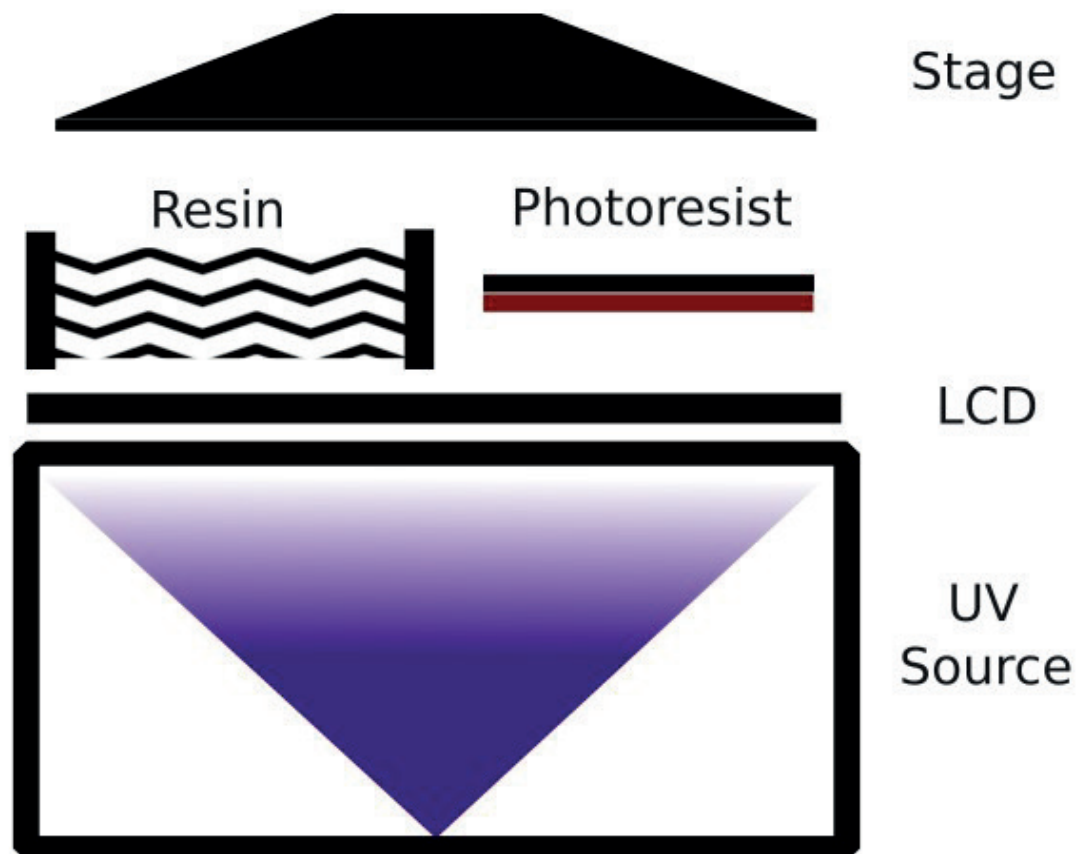
Low Cost Nano Lithography using Commercial 3D UV Resin printers

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As an alternative to expensive machines, this work develops a technique to perform photolithography using a commercial 3D resin printer: The Elegoo Mars 4[1] This allows for electrical devices to be fabricated with $\sim 20\mu\text{m}$ resolution at two orders of magnitude cheaper than many photolithography machines[2]. This work explores the possible applications of this technology as well as potential advantages it has over traditional photolithography methods.



Replacing printer resin with photoresist, the LCD converts the UV light shining on it to the pattern being exposed. This can resolve details on our substrates as fine as $20\mu\text{m}$ consistently, with easy operation.

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Tuning PDMS surface properties for Organ-on-chip devices applications

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Organ-on-a-Chip (OOC) technology emerges as a promising alternative to conventional 2D cell culture and animal experimentation in biomedical research. These devices offer significant potential for preclinical studies and drug development [1]. The construction of OOC devices involves integrating cell cultures and extracellular material within microfluidic compartments to replicate essential organ features, including cellular microarchitecture which includes nutrient perfusion channels resembling blood vessels. To manufacture a chip, a previously made master is replicated using polydimethylsiloxane (PDMS) which is later adhered to a glass to form a full device. PDMS has many interesting properties; it is a transparent material, inert and biocompatible. However, its strong hydrophobic nature possesses challenges when dealing with water-based biological reagents since it can affect fluid flow and cell adhesion. Hence, modifying its surface properties to enhance wettability [2] and facilitate fluid flow within channels will be highly beneficial for OOC technology. This work explores different modification routes to improve the surface hydrophilicity. We present a comparative study involving various modifications, wetting characterization, and biocompatibility assessments. Characterization of wetting properties using water contact angle (WCA) measurements was done on the distinct surfaces: PDMS, 2 copolymers mixed in pre-polymerization (PEG & tritonX100) and 2 coatings (PVA & PVP). This proved that all the surface modifications improved the wettability, with the best results given by the PVA and the PEG. Outcomes propelled us to explore the feasibility of introducing a fluorescent solution into micro-channels by capillarity. Cell viability essays are being performed using pancreatic tumor cells (MIA-PACA-2). The goal is the fabrication of a functional chip with modified PDMS to enhance properties of interest such as adhesion, biocompatibility wettability.

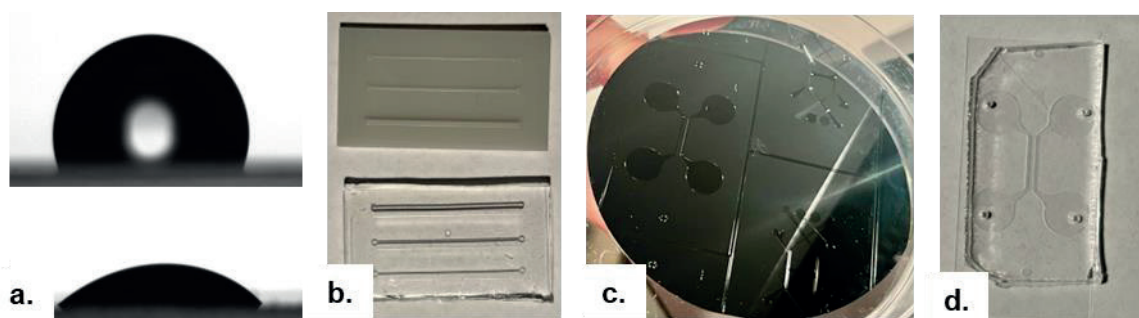


Figure 1: a) Difference in water contact angle (PDMS vs PVA) b) 3D printed mold and channels c) Silicon master mold d) PDMS chip.

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Influence of infrared blocker content on the thermal conductivity of microcellular PMMA.

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Polymer foams is a two-phase system composed of a solid polymer matrix and a gaseous phase. Microcellular polymer foams are characterized by a porous structure with a cell size in the range of the micrometers. These materials exhibit reduced weight to volume ratio, robust compressive mechanical properties and specially extremely good thermal insulation which makes them suitable for a variety of applications.

Nevertheless, there is potential for enhancing the thermal and mechanical characteristics of these materials. Because of their low density and pore dimensions, they exhibit minimal absorption or scattering of infrared radiation, thereby increasing overall thermal conductivity. One strategy to address this issue could involve incorporating opacifiers that serve as blockers against infrared radiation [1]. Moreover, these opacifiers have the potential to strengthen mechanical properties as well.

In this work carbon nanoplatelets (GnPs) have been added in different amounts between 0.5 and 10% of the total weight to different samples of PMMA with cell sizes in the range of 2 to 5 micrometers with relative densities among 0.1 and 0.2. The thermal conductivity of these materials has been measured and compared with microcellular PMMA samples without opacifiers in order to study which contents are the most optimal to reduce the thermal conductivity without altering the cell structure. A theoretical model [2] was used to determine the different contributions of solid, gas and radiation to the total thermal conductivity. It has been obtained that contents of GnPs in the range of 0.5 to 2% reduce in a 8% the radiative term respect to pure PMMA reaching values of total thermal conductivity of 38 mW/(m K). Therefore, this study presents a direct approach to enhance the performance of microcellular foams which can be extrapolated to other polymers.

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Acknowledgements

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Isorecticular Expansion and Linker-Enabled Control of Interpenetration in Titanium-Organic Frameworks

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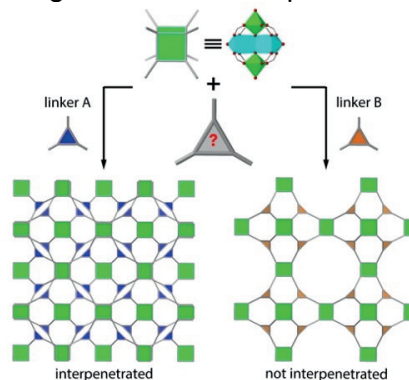
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Among many other fascinating features, the modular nature of reticular solids is one of the most attractive for the design of porous materials. In the case of Metal-organic frameworks (MOFs), this possibility is enabled by using inorganic polynuclear clusters known as secondary building units (SBUs) as nodes with predefined symmetry and connectivity. The structural information encoded in these nodes can be used to target the assembly of binary frameworks with “default” topologies by reaction with organic links and nodes provided their functionalization does not alter SBU formation. This provides a versatile playground for the rational design of isorecticular frameworks.^[1] However, this possibility is only accessible for a limited number of polynuclear clusters.

We recently reported the possibility of using the heterometallic Ti Cluster $[\text{Ti}_2\text{Ca}_2(\mu_3\text{-O})_2(\text{RCO}_2)_8(\text{H}_2\text{O})_4]$ (Ti_2Ca_2) to assemble two isorecticular **the** nets: MUV-10 and MUV-12.^[2,3] These results encouraged us to explore if this SBU might be used as a persistent node amenable to the reticular design of Titanium frameworks. In this study, we present two approaches in which we confirm that this cluster is fully compatible with the synthesis of isorecticular MUV-12(X) and MUV-12(Y) crystals with tailorable porosities and versatile pore chemistries. We also demonstrate how framework interpenetration can be overcome by introducing steric restraints to the peripheral 4-carboxyphenyl units of the linker for the assembly of non-interpenetrated structures with surface areas near to $3.000 \text{ m}^2\cdot\text{g}^{-1}$, the highest reported for titanium-based MOFs to date.^[4]



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Biocompatible Zn metal-organic frameworks for drug capture

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Metal-organic frameworks (MOFs) have undergone significant advancements in both biological (1) and environmental (2) fields, owing to their biocompatibility and capacity for pollutant capture. However, the full extent of their potential remains largely untapped. Hence, this project is dedicated to the development of biocompatible MOFs derived from amino acids serving as organic ligands, in conjunction with metals like Zn^{2+} and Ca^{2+} (as a secondary metal), with a specific focus on their application in drug delivery (Figure 1). The synthesis methodology entails direct preparation of the MOF, preceded by the synthesis of the organic ligand. Alternatively, these materials can be indirectly prepared starting from a Ni^{2+} precursor through a transmetallation process. Subsequent characterization involves a multitude of techniques including Powder X-ray Diffraction (PXRD), N_2 adsorption (ADS), and microanalysis (SEM-EDX), among others. Currently, the synthesis process has been set up, although further optimization of conditions is required to enhance their efficacy as drug carriers. Moreover, forthcoming plans involve conducting comprehensive scale-up tests to explore the potential applications outlined above.

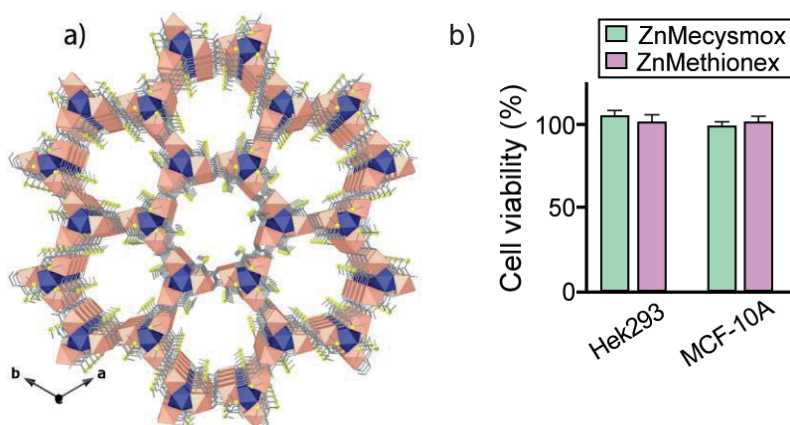


Figure 1. (a) Structure of $\text{Zn}_6\text{CaMecysmox}$. (b) Biocompatibility tests: Viability of MCF-10A and Hek293 cells after treatment with MOFs $\text{Zn}_6\text{CaMecysmox}$ and $\text{Zn}_6\text{CaMethionex}$ ($10\ \mu\text{M}$) which was assessed by MTT assay and expressed as a percentage respect to vehicle-treated cells.

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Design of novel Metal Organic Frameworks built from oxamate-functionalized amino acid ligands

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The principal aim of this study is to advance in the design and synthesis of metal organic frameworks (MOFs) with oxamate-based ligands derived from amino acids, a field that has experienced remarkable expansion in last years. To achieve this goal, we have selected functionalized oxamate derivatives to fabricate extended architectures capable of showcasing intriguing characteristics, such as chirality [1]. The synthesis process follows an indirect route, first the synthesis of the amino acid oxamate as ligand, followed by the formation of the Cu^{2+} complex, metalloligand, with the oxamate and finally the MOF is formed with $\text{Ni}(\text{cyclam})\text{Cl}_2$ as second metal. The characterization of the MOFs is performed by powder and single-crystal X-ray diffraction (PXRD and SCXRD), microanalysis (SEM-EDX) and N_2 or CO_2 adsorption. The synthesis conditions will be further refined to obtain the best ones and apply them to the separation of enantiomers taking advantage of the chiral capacity of amino acids.

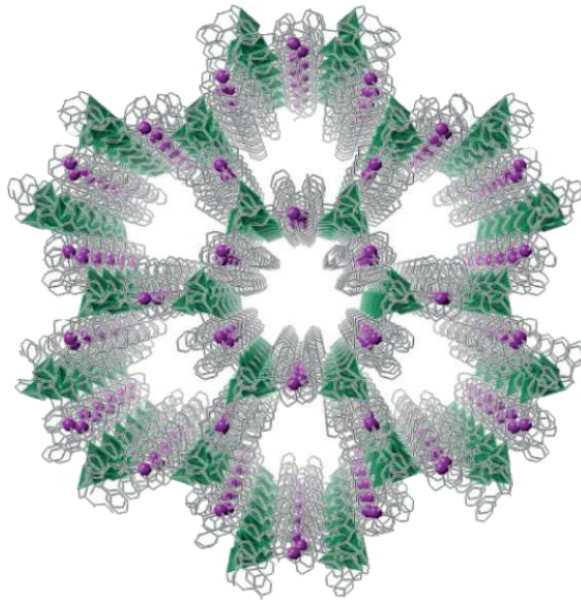


Figure 1. The copper(II) and nickel(II) atoms are represented by green polyhedra and purple spheres, respectively. The ligand backbone is depicted as grey sticks.

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Boosting protein encapsulation through Lewis-acid-mediated MOF mineralization: toward effective intracellular delivery

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In the last years, different Metal-Organic Frameworks (MOFs) have been explored as supports for the encapsulation of biomolecules, resulting excellent candidates for the immobilization of biomolecules¹ owing to their physico-chemical stability, their convenient biodegradability and the possibility of synthesis under biocompatible conditions. This last trait opens the possibility to the so called in-situ synthesis, that consists on the spontaneous assembly of protective MOF coatings onto the biomolecules. This strategy has been shown to depend on the effective interaction between the MOF precursors, mainly the metal cation, and the biomolecule surface, in some cases being hampered by its surface electrostatics.² Herein, we present a general in situ biomolecule encapsulation using a biocompatible MOF, the mesoporous trimesate iron-based MIL-100(Fe) material. We demonstrate that MOFs based on cations exhibiting considerable inherent acidity are suitable for biomolecule encapsulation regardless of their isoelectric points ($5 < pI < 11$), . MIL-100(Fe) scaffold retains protein activity and permits release under biocompatible conditions, allowing their use in desired biological applications.³

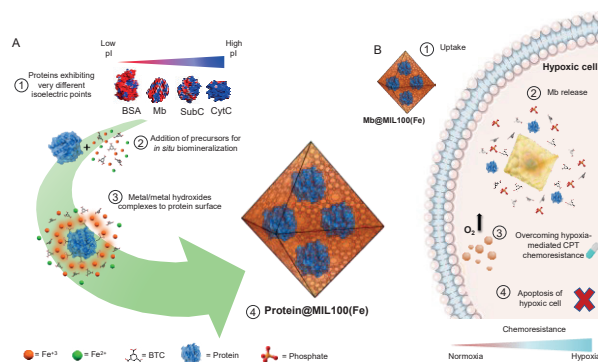


Figure 1: (A) Schematic representation of the in situ encapsulation of proteins in MIL-100. (B) Intracellular delivery of O₂ by myoglobin@MIL-100 composite and sensitization to chemotherapeutic agent.

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Solvent-Free Synthesis for Harvesting Novel Melting MOFs

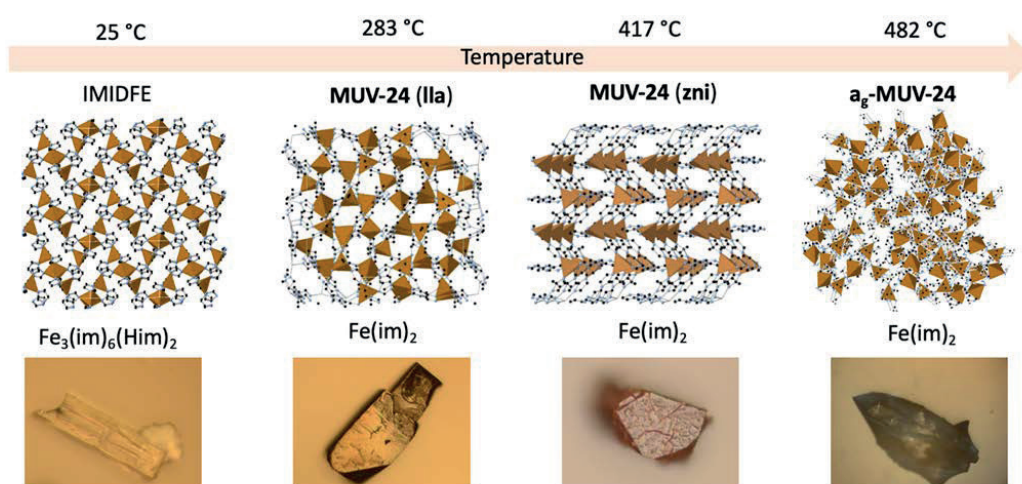
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Metal-Organic Frameworks (MOFs) are a family of porous crystalline materials formed by organic ligands and metal ions (or clusters). A subfamily within MOFs is that of zeolitic imidazolate frameworks (ZIFs). Recently, this family has shown to be able to reach a liquid state prior to material decomposition [1]. Furthermore, the glass formed upon vitrification of liquid phase retains the basic metal-ligand connectivity of crystalline MOFs, which connects their mechanical properties to their starting chemical composition [2]. So far only a handful of ZIFs capable of reaching the liquid phase have been reported, including ZIF-4 (cag), ZIF-62 (Zn and Co) and ZIF-76. The focus on the field is to find new materials capable of melting and in reducing the melting temperature (T_m) to increase its potential applications.

Thus, motivated by the prospect of expanding the family of ZIF glasses we explore the preparation of a novel Fe-glass in an indirect manner. We have successfully synthesized and characterized the first Fe-ZIF glass, denoted **a_g-MUV-24** [3], which is obtained via a three-step structural rearrangement from the known coordination polymer $[\text{Fe}_3(\text{im})_6(\text{Him})_2]$, in which octahedral and tetrahedral Fe(II) centres alternate. In the first step, a release of the terminal protonated imidazole ligand occurs, yielding a dense 3D solid with a new topology, denoted **MUV-24(IIa)**, with exclusively tetrahedral Fe(II) centres. The second structural transformation causes this solid to rearrange into the well-known zni topology, already reported for Zn(II) and Co(II), but not Fe(II). Finally, upon further heating **MUV-24(zni)** to 482 °C, the solid melts. This melting temperature for $\text{Fe}(\text{im})_2$ is significantly below the melting temperature of the Zn analogue, thus potentially improving the applicability of the material.



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MOF-on-MOF heterostructures for water splitting photocatalysis under solar light

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Metal-Organic Frameworks (MOFs) also known as porous coordination polymers (PCPs) are versatile materials that have revolutionized the field of porous solids materials during the last decades. Their hybrid modular nature, together with their unprecedented porosity are responsible of their multiple applications in very distinct fields including storage/separation, catalysis and drug delivery. Integration of different MOFs to construct hybrid MOF-on-MOF heterostructures has produced an emerging class of materials with tailored compositions and functionality.[1][2] These hybrid heterostructures have shown promising uses surpassing in some cases individual performances. However, control over the synergistic effects identified among individual MOF ingredients remains challenging. Herein we present the synthesis of hybridized MOF-on-MOF nanostructures obtained by epitaxial growth of flexible iron-based MIL-88B MOF onto the (111) facet of robust zirconium-based MOF nanoparticles of UiO-66-NH₂. Structure characterization reveals the retention of MIL-88B flexibility after the epitaxial growth. Finally, the UiO-66-NH₂@MIL-88B heterostructure exhibits higher photocatalytic performance under solar light for water splitting compared to the individual MOFs.[3]

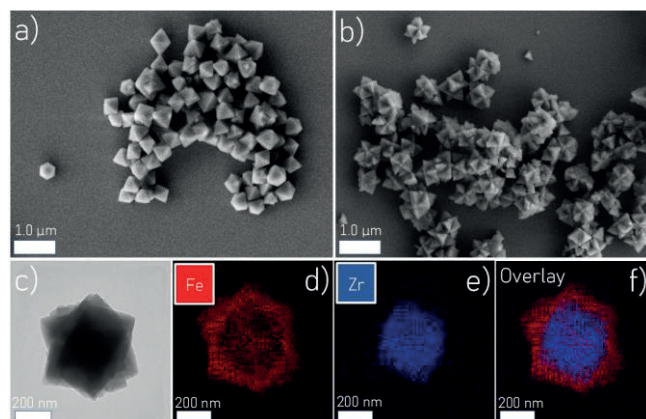


Figure 1. SEM images of a) UiO-66-NH₂ and b) UiO-66-NH₂@MIL-88B, c) HRTEM image of UiO-66-NH₂@MIL-88B and d,e,f) EDS mapping of UiO-66-NH₂@MIL-88B.

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Photo-organocatalytic Decarboxylative Borylation

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Boronic acids or esters are versatile functionalities in organic chemistry through which valuable building blocks can be obtained via cross-coupling, carbenoid or radical reactions. Notably, boronic acids are used in material chemistry for the synthesis of 2D and 3D metal organic frameworks (COFs) and they are also employed in medicinal chemistry as carboxylic acid bioisoters.^{1,2} Traditional pathways to access this kind of products include the use of organometallic reagents and Pd catalysts. Recently, methods involving radical decarboxylation have been developed due to the abundance of carboxylic acids, allowing for safer and milder reaction conditions. In general, these methods use expensive diboron reagents (namely B₂cat₂ and B₂pin₂) as boron sources in combination with metal catalysis (Cu or Ni), metal photocatalysis (Ir), metal electrocatalysis or direct photoexcitation.^{3,4} Herein, we disclose a new methodology for the synthesis of alkylboronic esters. This metal-free, light-initiated methodology uses an inexpensive diboron reagent B₂(OH)₄ in combination with catalytic amounts of widely available organocatalysts (catechol and pyridine) producing a variety of compounds with moderate to good yields.

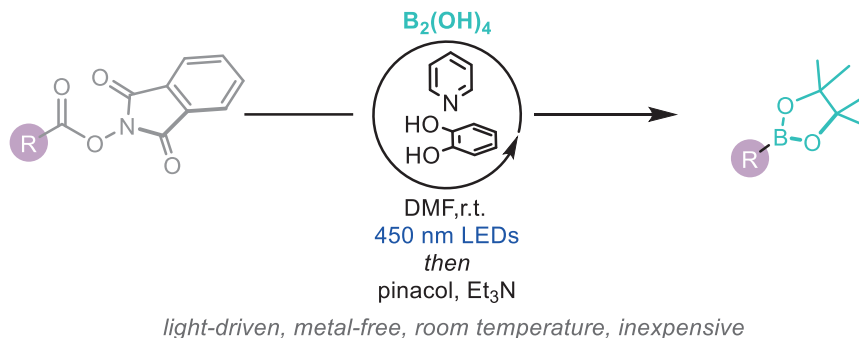


Figure 1: Photoinduced decarboxylative borylation

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Integrating Compositional and Structural Diversity in Heterometallic Titanium Frameworks by Metal Exchange Methods

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The synthesis of Metal-Organic Frameworks, MOFs, follows almost arithmetic principles based on the bonding points and symmetry of the organic and inorganic building blocks, and can yield a wide variety of crystalline porous solids with great structural and compositional diversity. In addition to increasing the diversity of MOFs by design, post-synthetic methods have also been developed to obtain materials that are in many cases inaccessible by direct synthesis.^[1]

This work deals with the experimental variables of the dynamic topological transformation, previously reported by the group, where a metal exchange induces a change in the topology of the material MUV-10(Ca) with “*the*” topology, to transform it into another different material, MUV-101(Co), with “*mtn*” topology.^[2] (Figure 1) During the optimization of the process, a new method is achieved to perform metal exchange without transformation, obtaining a new material, MUV-10(Co) (Figure 1). To extend the method, a new material is designed, MUV-30(Ca) (isoreticular to MUV-10), and the exchange and transformation are carried out, resulting in the materials MUV-30(Co) and MUV-301(Co) (Figure 1).^[3]

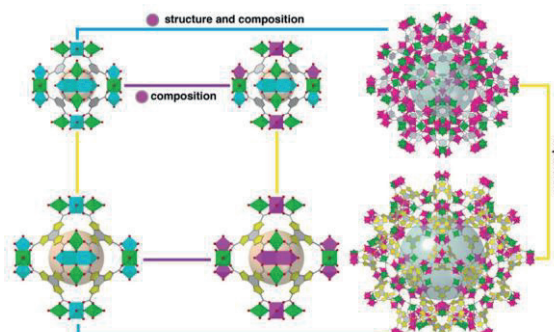


Figure 1: Diagram of the families of materials obtained in this work: btc family (top) and BTT family (bottom).

Finally, to validate the effect of ligand and metal substitution, the BTC-based material and the BTT-based material families were tested as photocatalysts in the hydrogen evolution reaction. The first surprising finding is that the incorporation of Co^{2+} has a negative effect. It is also noted that the ligand changes from BTC to BTT, i.e. from MUV-10 to MUV-30, is seen to be significantly improved, although it is also possible that this is due to the increase in pore volume.^[3]

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Ultrastable pyrazolate porphyrin metal-organic frameworks for environmentally relevant applications

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Metal-Organic Frameworks (MOFs) are highly porous crystalline architectures comprising organic linkers and inorganic metal nodes/clusters, offering unmatched structural and compositional versatility. MOFs synthesis often involves the reaction between organic linkers, typically carboxylate-based, metal salts, solvents, and modulators.

The incorporation of metals and porous structures renders MOFs particularly attractive for catalytic applications,^[1] such as electrochemical CO₂ reduction reactions (eCO₂RR). However, their stability under electrocatalytic conditions remains a significant challenge, particularly for prototypical carboxylate-based MOFs.^[2] Conversely, MOFs featuring pyrazolate (pz)-derived ligands and low-valent metal ions offer enhanced chemical stability potential for high-stability demanding reactions as eCO₂RR (**Figure 1a**). Despite the ability of pz-linkers to form topologies analogous to carboxylate ligands like carboxylate porphyrin MOFs (pf-MOF), examples of pz-MOFs are scarce and have seldom been tested in environmentally applications necessitating robust chemical stability.^[3]

As a start point for the use of MOFs in high-stability demanding applications, we have synthesized metal pz-porphyrin (pz-MPf) MOF PCN-601 [Ni₈O₆(pz-MPf)₃]^[3] and studied its stability under eCO₂RR conditions. As depicted in **Figure 1b**, X-Ray diffraction analysis (PXRD) remain excellent crystallinity across all samples following exposure to a 0.5M NaHCO₃ solution over several days.

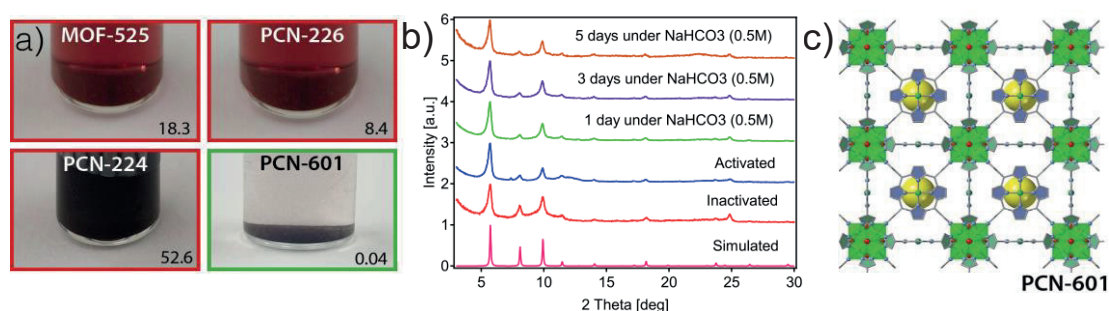


Figure 1. a. Porphyrin carboxylate MOFs (red) vs porphyrin pyrazolate MOFs (green) stability under NaHCO₃ (0.5M) buffers as the ones used in eCO₂RR. b. Experimental and simulated PXRD of PCN-601 under different conditions. c. Crystal structure of MOF PCN-601.^[3]

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Assessment of the interaction to G4s, nucleotides and drugs of novel G4 supramolecular binders

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Supramolecular structures such as capsules, cryptands or macrocycles are interesting systems for the selective recognition of small molecules and capable to transport cargoes through synthetic and natural barriers.^[1] These systems could be applied in drug delivery, pollution remediation, catalysis and in many other areas. Of outmost importance, the supramolecular systems could target biomolecules such as nucleic acids or proteins and exert a synergetic effect of the encapsulated molecule and the capsule itself.

Among the novel drug targets in drug discovery, epigenetic alterations, including histone modification, nucleosome remodeling and other non-coding mediated structures have attracted the attention in the last decades.^[2] One of the most attractive non-coding structures in anticancer drug development are G-quadruplex (G4) DNA and RNA. G4s are non-canonical nucleic acid structures formed in guanine-rich sequences.^[3] Strikingly, a large number of putative G-quadruplex forming sequences have been identified in the genomes of human, microorganisms and viruses, and the evidences suggest their pivotal role in key biological processes. Telomeres are regions enriched with putative G4-forming DNA sequences and have been associated to ageing and cancer. Telomere sequences comprise hundreds of TTAGGG repeats which form a superstructure constituted by multiple G4s, termed as multimeric G4s (multG4s). Therefore, multG4 structures are currently tested as a therapeutic target to block telomere elongation in cancer cells.

Herein, we present the interaction of a series of macrocycle and cryptand-like systems with G-quadruplex DNA located at proto-oncogenes and telomeres by a high-throughput fluorescence displacement assay (HT-FID). We then evaluated the interaction of these systems with anticancer drugs and nucleotides by potentiometry in order to assess the capacity to transport them through cell membranes and deliver the cargo. Our theragnostic approach could be then applied to target the telomeric/oncogenic regions and other cancer-related pathways associated to the drug encapsulated.

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A radio frequency study of magnetic nanoparticles deposited on solids for sensing applications

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Magnetic nanoparticles are excellent candidates for labeling and detecting biomarkers in rapid diagnostic tests such as lateral flow immunoassays [1]. However, this type of test requires a good capillary flow of the bioconjugates along the membrane, thus limiting the size of the nanoparticles and the bioconjugates. A study of magnetic nanoparticles deposited on solid substrates could open the door for developing static immunoassays such as an ELISA. Therefore, bigger-sized magnetic nanoparticles could be used, contributing to a larger sensitivity and binding range. It could also be used for the measurement of magnetic nanoparticles inside cells. In this work, we designed and optimized a new measurement system using a refractometry and radiofrequency sensor [2]. We synthesized magnetic biofunctional nanoparticles based on manganese ferrites using the hydrothermal coprecipitation method. Finally, we deposited the synthesized magnetic nanoparticles in a solid substrate and quantified their signals. We obtained calibrations with a R^2 of 0.9995, and with a very big signal-to-noise ratio for this type of measurement. Therefore, our results support the promising use of this new measurement system for sensing applications.

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Mesoporous nanocatalysts based on Pd for biorthogonal chemistry

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Coined in 2003 by the 2022 Chemistry Nobel Laureate Carolyn R. Bertozzi, the term “biorthogonal chemistry” refers to reactions that allow for the chemical alteration of intricate biological molecules within their natural surroundings. These reactions do not have natural equivalent and/or inherent reactivity with natural components [1], what makes them especially useful in the Nanomedicine field. It is here where the use of non-biotic Pd is on the rise, as its effectiveness for anticancer treatments based on the activation of prodrugs has offered promising *in vitro* results [2]. Nevertheless, it must be highlighted that despite its remarkable effectiveness, Pd typically suffers from biocompatibility, stability, or toxicity issues.

Taking all this into consideration, in this research, firstly, SiO₂ spherical cores were synthesized. With the aim of embedding the metal into them, the cores were functionalized with amine groups that strongly bond to the SiO₂, creating SiO₂@NH₂ nanoparticles. Next, Pd nanoparticles around 5nm size were embedded into the SiO₂@NH₂, resulting in the desired SiO₂@Pd. In order to avoid toxicity due to the leakage of PdNPs, or the entrance of large biomolecules that could passivate the catalytic surface chemical groups or react with them, the Pd nanoparticles were encapsulated within a mesoporous silica shell leading to nanocatalysts SiO₂@Pd@mSiO₂.

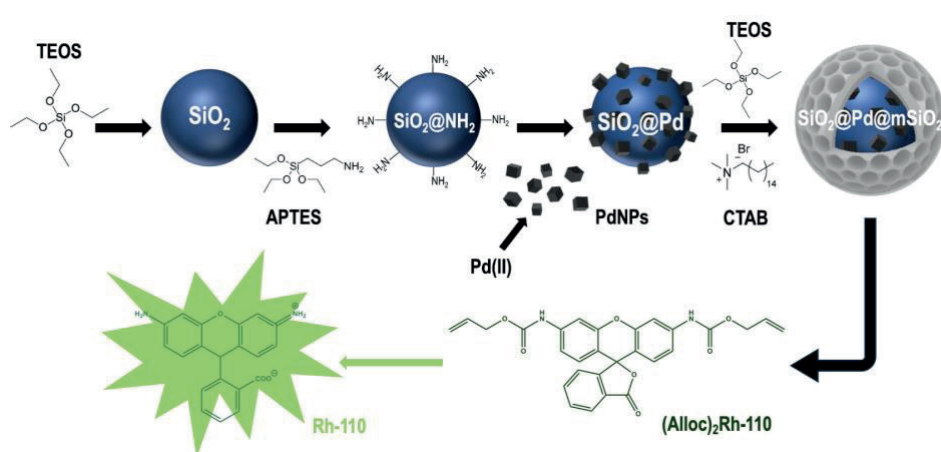


Figure 1. Scheme of the experimental process for the synthesis of the SiO₂@Pd@mSiO₂ nanocatalysts, and the catalytic deprotection of (Alloc)₂Rhodamine-110.

The resulting SiO₂@Pd@mSiO₂ nanoparticles have exhibited a pronounced catalytic activity for the deprotection of a fluorescence dye at low concentrations in physiological media.

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Harnessing Metal-Organic Frameworks for multi-contaminant water treatment and antibacterial action

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Water contamination is a pressing global issue with significant implications for human health, ecosystem integrity, and socioeconomic development. In response to this challenge, metal-organic frameworks (MOFs) have emerged as promising materials for various applications, particularly in water purification.[1] Among these, MOF-808 has attracted attention for its exceptional surface area and stability, while the presence of unsaturated metal sites in its structure make it an ideal candidate for functionalization to enhance its capabilities.[2]

In this work we present the synthesis and characterization of MOF-808 functionalized with nickel thiosemicarbazone complexes. The synthesis process involves preparing the organic ligands and their complexes with nickel ions and incorporating them into MOF-808 through post-synthetic modification. Thiosemicarbazone compounds exhibit remarkable affinity for heavy metal ions commonly found in aqueous environments. In addition, their complexes can also show antimicrobial activity against drug-resistant pathogens which also compromise global health.[3] On this basis, these advanced functionalized materials could have important application potential for sustainable processes such as water decontamination or as drug resistant pathogens.

Characterization techniques such as powder X-ray diffraction (PXRD), elemental analysis, ¹H NMR and Fourier-transform infrared spectroscopy (FTIR) have been employed to confirm the successful synthesis and integration of the compounds within the MOF. Initial results are also presented on the release of nickel species from the complexes in water and in biological buffers. Overall, this research contributes to the development of advanced materials towards important environmental- and health-related challenges.

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Post-functionalization of Covalent Organic Frameworks aerogels

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Covalent Organic Frameworks (COFs) are materials of high interest for a great variety of applications in the modern world due to their designability, porosity and tailorable properties. Ever since their discovery, COFs have been primarily synthesized through the solvothermal method, which implies high consumption of energy and low processability^[1]. COF aerogels have been reported as an alternative, presenting not only enhanced processability, but also hierarchical porosity and very low density^[2], which makes them especially appealing for electrodes of supercapacitors and batteries.

To excel in this application, COF aerogels need to improve their low conductivities by integrating highly conductive materials^[3]. Hence, in this presentation, we show a method to obtain a thiol functionalized COF^[4] able to host conductive nanostructures. The COF aimed for is achieved after several post-synthetic modifications on the COF-gel, preserving the processability showed by the original gels and aerogels. Characteristics such as crystallinity, porosity and composition of the intermediates and the final aerogels will be studied to prove the success of the reactions.

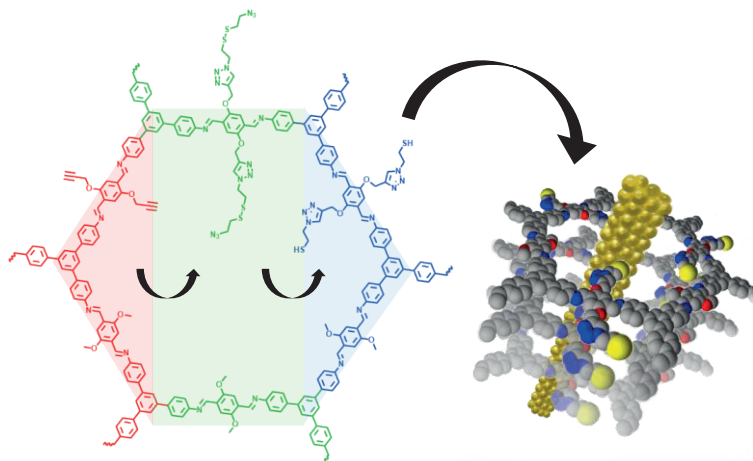


Figure 1. Post-synthetic modifications on COF gel for conductive nanowire incorporation.

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Removal of pharmaceutical pollutants by hydrogels of Covalent Organic Frameworks

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Pharmaceutical products are an important class of emerging pollutants which are present in the environment as a consequence of their production and formulation, patient use and improper disposal. They are typically found in the aquatic environment in concentrations from sub-ng/L to a few $\mu\text{g/L}$.^[1] This leads to the contamination of water supplies or local sources used by nearby communities or wildlife. As a consequence, it is necessary to develop new and efficient technologies for water remediation. In this context, porous materials have gained enormous research consideration for wastewater treatment. Covalent Organic Frameworks (COFs) are a new class of crystalline porous materials based on the integration of organic building blocks into an ordered structure.^[2] Benefiting from the features of designable regular porous structures and versatile functionalities, COFs have shown promising properties in adsorption of contaminants.^[3]

This communication describes the development and characterization of a two-dimensional COF based on imine bonds, named as TAPB-DBBA-COF, following a 'sol-gel method'.^[4] Solvent exchange gives rise to the production of the material in its hydrogel form, which is explored for water remediation. The material offers high performance towards the capture of the pharmaceutical pollutants' propranolol and naproxen, both in batch and under flow conditions (Figure 1). The findings suggest that COFs-based hydrogels have the potential to significantly improve water treatment technology and address the issue of water pollution.

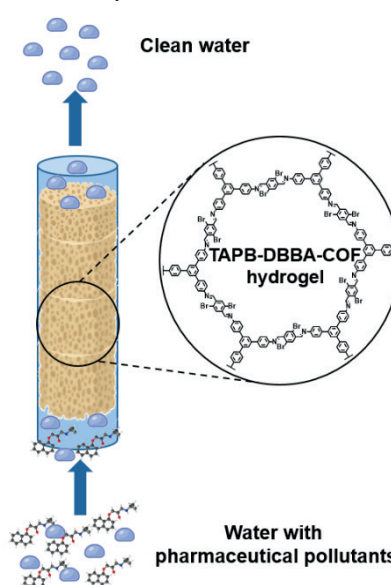


Figure 1. Drugs capture under flow conditions by using TAPB-DBBA-COF hydrogel.

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Synthesis of a perylene-3,4,9,10-tetracarboxylic diimide-galactose-phenanthroline conjugate for cancer therapy

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Perylene-3,4,9,10-tetracarboxylic diimides (PDIs) are typical semiconducting organic small molecules that possess highly interesting electronic and photophysical properties. After proper chemical modifications, PDIs have been widely used in electronic and optical applications, such as organic photovoltaic cells, dye lasers, organic field effect transistors, electronic memory devices, optical power limiters, and so on [1]. However, the growing interest on their use in biological studies in recent years, has promoted them to be considered as very promising molecules for research in the fields of Biology and Medicine [2]. Thus, for example, coordination of PDI with silver or copper ions has been shown to enhance anticancer activity by inducing apoptotic cell death [3].

However, PDIs have a limited solubility in water, therefore, we propose to synthesize new molecules with an improved design to increase both, the solubility of the complex and its internalization capacity inside the cells, with the objective to study their cytotoxic capacity against different tumoral cell lines.

In this work, we will present two molecules (Figure 1) with an improved design containing oligo (ethylene glycol) chains in an imide position and galactose rings in the bay region to ensure both water solubilization of the compound and internalization through active transport processes, in addition to 1,10-phenanthroline on the other imide position, responsible for metal chelation.

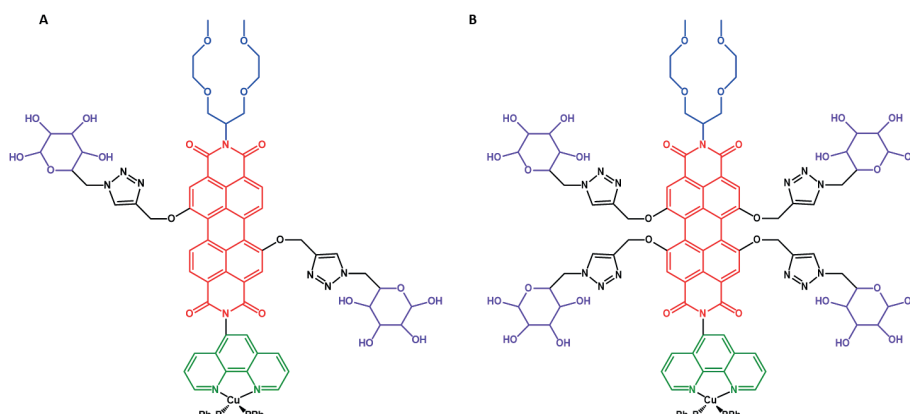


Figure 1. Structure of perylene-3,4,9,10-tetracarboxylic diimide-galactose-phenanthroline conjugates

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Elastin-like recombinamers hydrogels: Sinergistic combinanntion of thermal responsiveness and bioactivity on celullar response

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Elastin-like recombinamers (ELRs, recombinant protein polymers inspired on the intrinsically disordered domains of natural tropoelastin) have emerged as a promising component in tissue engineering due to its exceptional elasticity and biocompatibility and by the possibility of control their composition at the gen level by genetic engineering techniques. In this study, we explore the application of tailored designed ELRs in generating hydrogels via click chemistry, highlighting its ability to form stable three-dimensional networks. We investigate the temperature sensitivity of these hydrogels, revealing thermo-responsive properties that allow precise control over the structure and stiffness of the material.

Furthermore, we evaluate the incorporation of cell adhesion sequences to enhance cell interaction. Through in vitro assays, we test cellular behavior on these modified substrates, observing increased cell adhesion and proliferation compared to conventional substrates.

Our findings suggest that ELR hydrogels, generated via click chemistry, represent a versatile and promising platform for biomedical applications. The combination of their temperature sensitivity and ability to promote cell adhesion clearly enhances cell material interactions and, therefore, offers new opportunities in tissue engineering and cellular regeneration.

New styryldiazepinoporphyrazines from CCMoids for coordination polymers

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Keywords: *curcuminoids, phthalocyanines, coordination polymers, 2D molecular-based materials*

2D coordination polymers (2D-CPs) containing conjugated frameworks present interesting electronic properties with potential applications in areas such as optoelectronics and sensing, due to the conductivity, low dimensionality, high surface area and ordered arrangement of active sites in their structures^[1]. The use of conjugated and planar ligands, such as curcumin derivatives, the so-called curcuminoids (CCMoids), has been recently described for the construction of bioMOFs (Metal-Organic Frameworks)^[2] and 1D-3D CPs^[3]. This way, CCMoids have been used as organic linkers to bind to metal centers or clusters forming infinite structures^[2,3], due to the presence of three coordinative points in their structure (the β -diketone group and the aromatic ring substituents in lateral positions). Another exceptional family of organic systems are phthalocyanines (Pcs), which are planar macrocyclic structures, formed by four isoindole units connected by four nitrogen atoms, forming an inner ring with alternating carbon and nitrogen atoms. Peripheral modifications in these compounds increase the conjugation of the formed macrocycle and also allow their coordination with metals or other organic compounds, forming 2D coordinated and/or extended covalent structures^[1,4].

In this work we focus on the synthesis and characterization of Pcs from CCMoids and their derivatives for their potential application in coordination polymers.

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Nanozymes Mimicking Superoxide Dismutase: An Outstanding Antioxidant Performance

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The malfunction of the nervous system associated with several neurodegenerative disorders has been linked to the misregulation of free metal ions and oxidative stress. For example, in Alzheimer's disease, the accumulation of Fe and Cu in beta-amyloid plaques is thought to be responsible for increased oxidative damage in certain areas of the brain. These transition metals promote the aggregation of protein fibrils into peptide aggregates and mediate the production of reactive oxygen species (ROS) through Fenton reactions, with superoxide radicals playing a major role. Ongoing research is focused on the chelation of these redox active transition metals to avoid their participation in the formation of the peptide aggregates, as well as on the reversion of their activity from ROS generation to antioxidant activity. [1]

A family of tetraaza-pyridinophane macrocycles capable of chelating Fe(II) and Cu(II) has been synthesized and characterized. Potentiometric and UV-Vis titrations, along with superoxide dismutase and H₂O₂ removal activity assays, indicate that the synthesised macrocycle can coordinate Cu(II) and Fe(II) at physiological pH, resulting in the formation of complexes with remarkable SOD activity and a significant capacity to scavenge H₂O₂ from solution, respectively. [2]

Boehmite nanoparticles (BNP) were functionalised with the synthesised tetraaza-pyridinophanes and the resulting systems were characterised by NMR, elemental analysis, ICP-MS and DLS. The studies showed the nanostructured systems had up to 5-fold increased SOD activity, with regard to the non-anchored complexes. This might be attributed to the positive z-potential of the BNP, which would attract the anionic substrates towards their surface. [3]

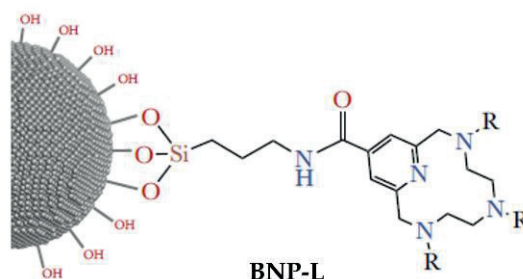


Figure 1. Family of nanozymes synthesized and studied.

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Voltammetric MIP (Molecularly imprinted polymer) sensor for sugar detection using nanoparticle and chitosan.

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In recent years, voltammetric sensors have been commonly used for assessing the electrochemical characteristics of an analyte. They are very helpful for investigating biological processes, tracing chemical substances, and differentiating the properties and functions of diverse systems. In the field of electrochemical sensors, molecularly imprinted polymers (MIPs) are widely used. Their high selectivity, anti-interference capability, and stability make them influential in studying different types of analytes following advanced sensor development. The ability of MIPs to create voids by eliminating template molecules is essential for the detection of analytes [1]. These interactions result in reactions like enzyme-substrate binding.

In this study, voltammetric sensors were designed to detect glucose and lactose. Both saccharides are abundantly present in the biotic environment. In biological systems, glucose serves as the primary energy source. The detection of glucose is vital for diabetes research, while analysing lactose plays a key role in developing safe dairy products. The goal of this research is to test whether integrating metallic nanoparticles based on silver (Ag) or gold (Au) can enhance the functionality of chitosan MIP sensors [2]. For this, nanomaterials are incorporated into highly biocompatible chitosan polymers to stabilise the matrix [3].

According to the obtained results, the high affinity and selective binding of MIPs make voltammetric sensors strong candidates for various applications in food safety and other industries. Furthermore, biocompatible polymers are a safe instrument for medical diagnosis because of their biodegradability, biocompatibility, and antibacterial characteristics.

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Enhancing chitosan based MIPs capabilities for wine compounds.

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Organic acids, recognized for their antioxidant, antimicrobial, and anti-inflammatory properties, are pivotal in various applications. In winemaking, where acidity levels are critical, monitoring and quantifying these acids is imperative. For this subject, electrochemical sensors provide fast, accurate and low cost analysis that would help winemakers to determine the final flavour and quality of a wine. Molecular Imprinted Polymers "MIP" are synthetic recognition materials designed with binding sites customized to fit specific template molecules, which ensures precise recognition.^{1,2}

By means of cyclic voltammetry, MIP sensors have been developed for various organic acids present in wine such as lactic, malic and tartaric acid. These sensors have been synthesized using Chitosan (CS), a biocompatible polysaccharide. Also, metallic nanoparticles (MNPs) can be added in order to increase the conductivity of the sensor. More precisely, silver nanoparticles (AgNPs) have been added successfully to the CS solution in different proportions to improve the sensibility of the sensor, due to the synergistic effect that MNPs have with chitosan.^{3,4}

The electrodeposition of Chitosan in a glassy carbon electrode via cyclic voltammetry allows to obtain electrochemical sensors for the detection of different organic acids that are present in wine. MIP chitosan based sensors are capable of detecting selectively different compounds, without the use of specific biological compounds, and in contrast with them, they can be easily prepared. All of this make them a very suitable choice for the detection of multiple compounds in the food industry.

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A Mechanosensitive Naphthalenophane as Platform for Quantum Interference Studies

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Mechanically induced destructive quantum interference is a feature known to be found in certain paracyclophane structures[1,2]. When such structures are prone to mechanical deformation, a particular configuration of the molecule can be probed, in which the frontier orbitals of the molecule overlap in such a way that the conductance is significantly suppressed. Using Mechanically Controlled Break-Junction (MCBJ) or Scanning Tunneling Microscopy Break-Junction (STM-BJ) techniques this quantum interference dip can be probed at room temperature and shows up in modulation experiments where the electrode separation distance is periodically increased and decreased (stretching and compressing the molecule), after which those individual dips can be used for statistical analysis. Here, we present the study of a naphthalenophane. Due its rigidity and high conductance it provides a versatile platform to not only study the mechanical dependence of the destructive quantum interference, but also for simultaneous thermoelectric measurements (using STM-BJ) and measurements at low temperatures (using MCBJ). We observe that the average thermoelectric response of the molecule does not change sign when crossing the quantum interference dip[3], which can be explained through the importance of several orbitals or transmission eigenchannels for quantum transport. On top of that thermal fluctuations show to play a role in suppressing quantum interference features.

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Ce(III)-Pt(II) coordination networks as magnetic luminophores sensitive to solvent vapors

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Coordination frameworks based on lanthanide(III) complexes are the subject of extensive research in recent years due to their diverse photoluminescent properties, including multi-colored emission sensitive to external stimuli such as solvent vapors or temperature variation. They are also widely examined due to their strong magnetic anisotropy that can lead to the Single-Molecule-Magnet (SMM) behavior. Therefore, due to the variety of optical and physical properties, this type of molecular material is considered for applications in various technological branches, such as high-density storage, chemical sensing, and luminescent thermometry.^[1-3] In this regard, we present a series of coordination frameworks based on Ce(III) complexes and tetracyanido-platinate(II) ions, including three-dimensional coordination networks, $\{[\text{Ce}^{\text{III}}(\text{MeOH})_2]_2[\text{Pt}^{\text{II}}(\text{CN})_4]_3\} \cdot 4\text{MeCN}$ (**1**) and $\{[\text{Ce}^{\text{III}}(\text{H}_2\text{O})_2]_2[\text{Pt}^{\text{II}}(\text{CN})_4]_3\} \cdot 4\text{H}_2\text{O}$ (**2**), as well as coordination layers, $\{[\text{Ce}^{\text{III}}(\text{H}_2\text{O})_6]_2[\text{Pt}^{\text{II}}(\text{CN})_4]_3\} \cdot 7\text{H}_2\text{O}$ (**3**), combining solvent-vapor-dependent SMM characteristics with guest-molecule-dependent multi-colored emission (Figure 1).

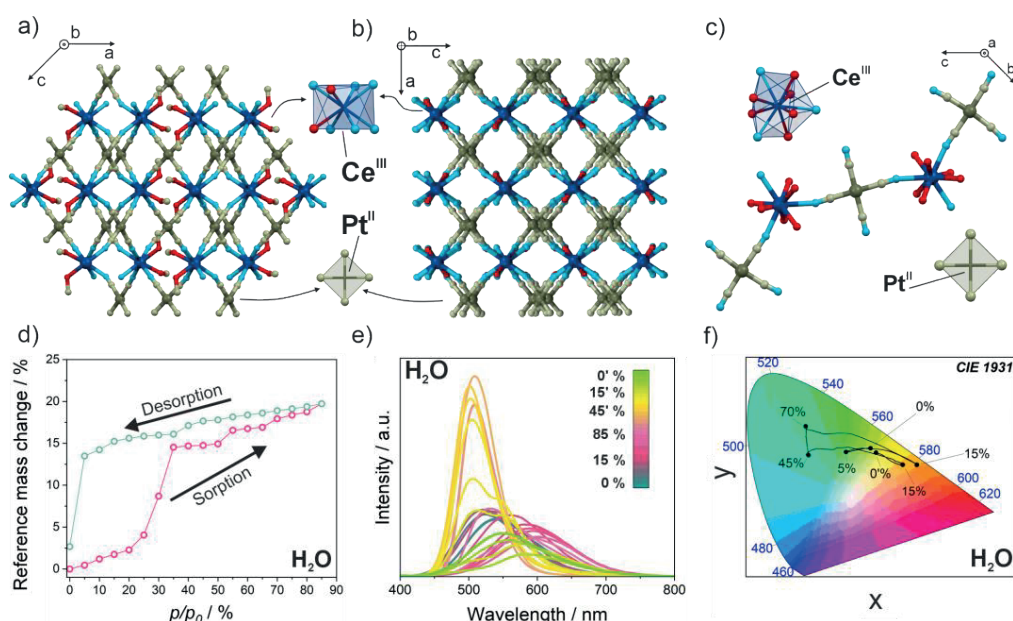


Figure 1. Representative structural fragments of **1** (a), **2** (b), and **3** (c); water sorption isotherm of **3** in the 0–85% relative humidity (RH) range (d); emission spectra of **3** collected in the 0–85% RH regime during the sorption-desorption cycle (e), and changes in emission visualized on the CIE 1931 chromaticity diagram (f).

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Optically pure propeller-shaped lanthanide single molecule magnets with helicene ligands

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In response to the rapidly growing demand for new technologies, single molecule magnets (SMMs) appear to be very promising candidates for ultra-high density data storage and fast information processing. Moreover, combining the magnetic memory effect of SMMs with other properties like optical activity opens new avenues towards modern molecular materials. A group of lanthanide complexes $\{\Delta\text{-}[\text{Ln}(\text{phendo})_4]\}\{\Delta\text{-}[\text{As}(\text{cat})_3]\}_2(\text{NO}_3)\cdot 5\text{MeCN}$ (Ln = Gd, Tb, Dy, Ho, Er, Tm, Yb) and (Λ,Λ) enantiomer ($\Delta,\Delta\text{-LnAs}$ and $\Lambda,\Lambda\text{-LnAs}$) with the smallest helicene-type ligand, 1,10-phenanthroline-*N,N'*-dioxide (phendo) [1] were obtained as pure enantiomers. Successful isolation of the left- and right-handed compounds was performed by their crystallisation with enantiomerically pure tris(catechol)arsenate(V) $\Delta\text{-}$ or $\Lambda\text{-}[\text{As}(\text{cat})_3]$ counterions [2]. The products were characterised using single crystal X-ray diffraction, magnetic measurements and natural circular dichroism (CD) spectroscopy. For selected analogues, magneto-chiral dichroism (MChD) measurements were performed, showing existence of the cross-effect arising from combining chiral and magnetic properties in a single molecule. The results allow to qualify described systems to the narrow group of helicene based materials showing magneto-chiral dichroism [3] and makes their further investigation even more captivating.

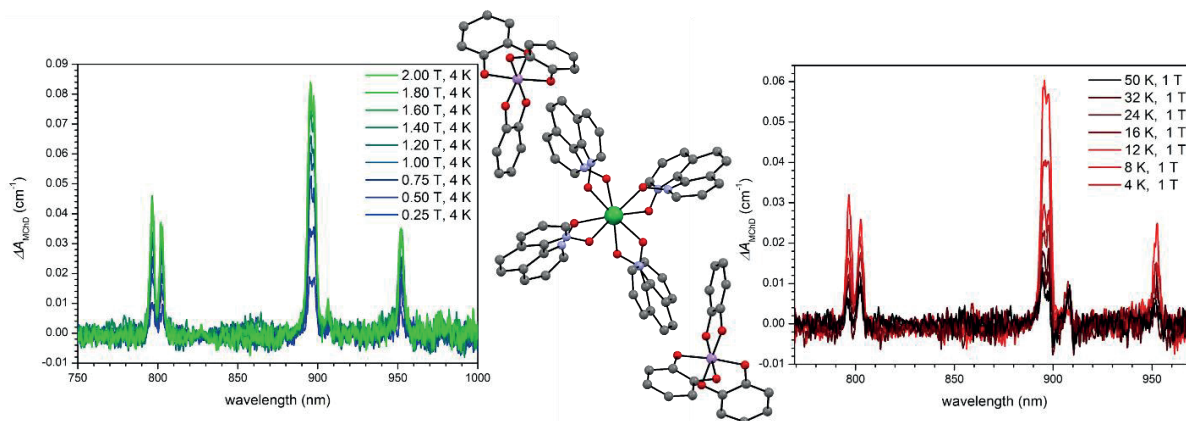


Figure 1. Crystal structure of $\Lambda,\Lambda\text{-DyAs}$ (middle; MeCN molecules and H-atoms omitted) and MChD spectra presented as a function of magnetic field (left) and temperature (right).

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Dielectric relaxations and photoluminescent properties in ionic salts based on the dicyanido-bis(2,2'-phenylpyridinate)rhodate(III) anion

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One of the aims of the state-of-the-art engineering of molecular materials is combining diverse physical properties in a single-phase material. Such properties include ferroelectric behavior, single-molecule magnetism, and photoluminescence, the implementation of which is mostly realized through the self-assembly of specific molecular building blocks. Among the wide array of building blocks that enable the creation of multifunctional molecular materials, polycyanidometallates and lanthanide ions are commonly used to introduce photoluminescence, meanwhile, the presence of organic polar cations induces thermally switchable dielectric properties that can lead to ferroelectricity.^[1,2] Through this approach, the molecular materials field has seen a rise in optoelectronic devices as well as tunable chemical sensors and actuators, sensitive to external stimuli applied to the materials.^[3]

In the course of our work, we obtained a series of molecular hybrids based on the dicyanido-bis(2,2'-phenylpyridinate)rhodate(III) anion and N-alkylated dabco (1,4-diazabicyclo[2.2.2]octane) derivatives of varying alkyl chain lengths (C₁-C₄) with the general formula of [R(dabco)][Rh^{III}(CN)₂(ppy)₂] (R = CH₃- (1), C₂H₅- (2), C₃H₇- (3), C₄H₉- (4)), exhibiting pronounced LMCT-based (ligand-to-metal-charge-transfer based) photoluminescence co-existing with switchable dielectric properties (Figure 1).

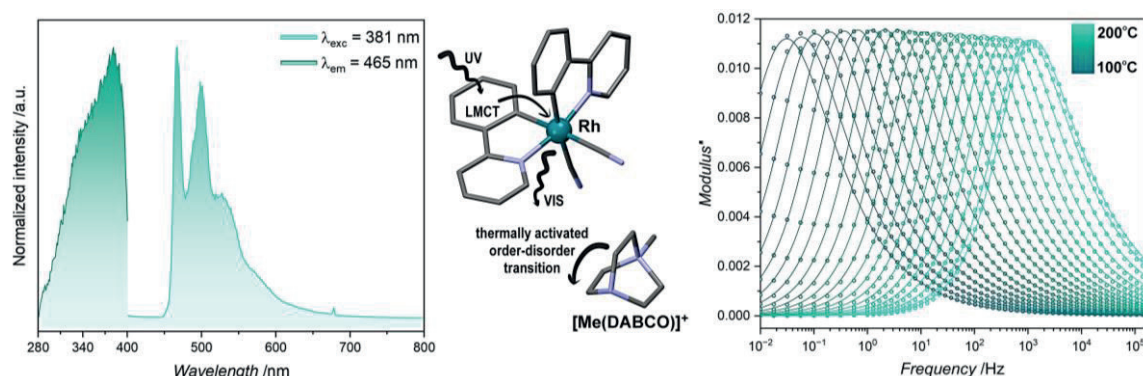


Figure 1. The asymmetric unit of **1** (center) along with its luminescent properties at 77 K (left) and the temperature-dependent dielectric relaxations under the ac electric field (right).

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Heterometallic s-d frameworks with hexacyanidometallates for the construction of luminescent sensors

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Luminescent materials exhibiting emission characteristics sensitive to temperature, relative humidity, or chemical stimuli have gained broad scientific attention in the last few years due to possible sensor applications. Such interest is governed by the aim of obtaining less invasive sensing methods with a relatively short time of the system's response. In these regards, a promising class of stimuli-responsive luminescent solids is formed by metal-organic frameworks (MOFs), i.e., crystalline porous materials constructed using coordination chemistry, which can exhibit photoluminescence (PL) originating from incorporated metal ions, organic linkers, or even guest molecules.[1-2]

To contribute to this field, we present a series of heterometallic MOFs (abbreviated below as **M1M2**) based on divalent s-block metal ions, $M1^{2+}$ ($M1 = Ca, Sr, Ba$), organic linkers of 4,4'-bpdo (4,4'-bipyridine N,N'-dioxide) and hexacyanidometallate anions, $[M2^{III}(CN)_6]^{3-}$ ($M2 = Co, Cr$). The **CaCo**, **CaCr**, **SrCo**, and **SrCr** systems crystallize analogously, forming 3-D coordination networks based on s-block metal ions bridged by 4,4'-bpdo ligands, with hexacyanidometallate ions and solvent molecules located in the pores of the rigid scaffold. On the other hand, the presence of larger Ba^{2+} ions results in the formation of **BaCo** and **BaCr** systems, where the hexacyanidometallates moiety is coordinated to the Ba^{II} centers. Among the series, the **SrCr** framework deserves special recognition due to its distinct and fully reversible water sorption as well as humidity-sensitive PL. The lifetime of the emission at 810 nm decreases in the wide range from 19 ms down to 1 ms at room temperature upon increasing relative humidity from 0 to 90%. Moreover, the strong temperature dependence of PL has also been noticed, which is mainly related to the strong enhancement of 4,4'-bpdo centered emission upon decreasing the temperature down to 10 K. Both features make the **SrCr** system a promising candidate for a multifunctional optical sensor.

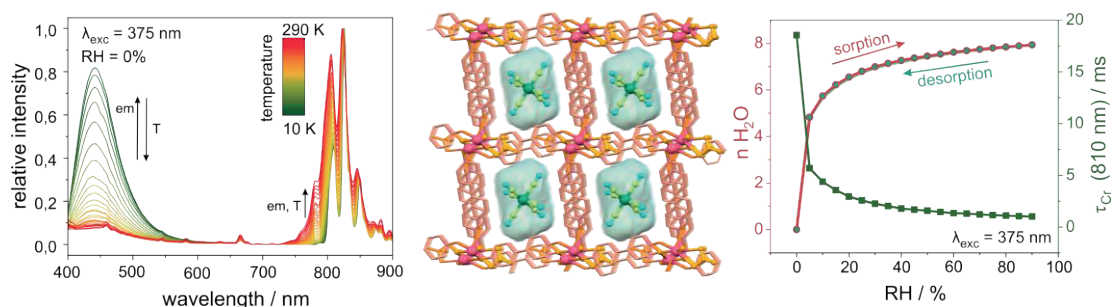


Figure 1. Fragment of the **SrCr** system with the outlined pores occupied by $[M^{III}(CN)_6]^{3-}$ ions (center). The T-variable emission spectra (left) and RH-dependent PL lifetime with a water sorption isotherm (right).

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DETECTION OF THE TWO-DIMENSIONAL VALENCE BOND SOLID STATE WITH SCANNING TUNNELING SPECTROSCOPY

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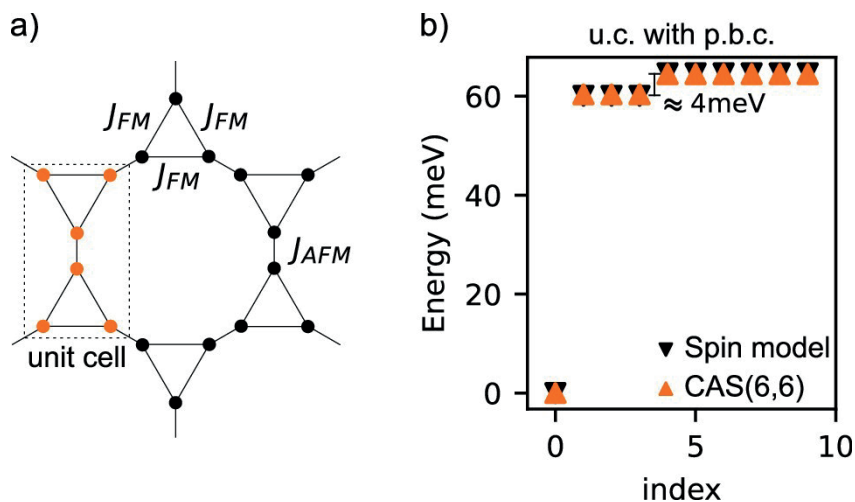
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The AKLT model plays a prominent role in the study of quantum magnetism. In 1D, the AKLT model provides a paradigmatic case of exactly solvable Hamiltonian with a topological phase. In two dimensions (2D), particularly in the case with $S=3/2$ spins on a honeycomb lattice, it manifests a unique ground state with a gap, representing a valence bond solid. This ground state has proven to be a universal resource for measurement-based quantum computation [2].

For a hypothetical finite-size system described within a general class of models with both linear and non-linear couplings, we investigate how to determine if it conforms to the AKLT model using inelastic tunnel spectroscopy implemented with scanning tunnel microscopy (IETS-STM). We propose two approaches: for a dimer, utilizing non-equilibrium IETS-STM to acquire various excited states and deduce both linear and non-linear exchange interactions. In the case of finite-size clusters, we argue that edges host zero modes, that could give rise to Kondo.

The use of Neural-Network Quantum States (NNQS) for deriving such ground states numerically for larger systems and the potential of nanographene based structures to obtain such models [3] is also briefly discussed.



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Sublimed Textured Tandem Silicon/Perovskite Solar Cell

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The progress in single-junction perovskite-based photovoltaic devices has been impressive over the last 14 years. Currently, the highest efficiencies for perovskite-based solar cells were obtained in tandem configuration combining solution-processed perovskite cell at the top and fully textured crystalline silicon at the bottom cell. Texturizing the Si bottom cells leads to enhanced light absorption and therefore higher current density and power conversion efficiency. However, it is more challenging to deposit the perovskite on the pyramidal texture resulting in non-uniform coverage and hence lower device performance. Among other merits, such as thickness and position tunability vapor-based deposition offers the viability of a more conformal and uniform deposition over textured surfaces.^[1]

Yet, it is not trivial to obtain fully covered interfaces which are needed for high efficiency perovskite cell performance. Furthermore, the analysis and optimization of perovskite-Si tandem cells is complicated as both subcells interact and contribute simultaneously to overall performance.^[2] In this work, we present a route towards optimization of tandem silicon/perovskite solar cells by using the textured Si cell only as the substrate instead of as the device. This allows us to characterize and improve the top perovskite cell as a single-junction cell only and to compare its performance with tandem solar cells.

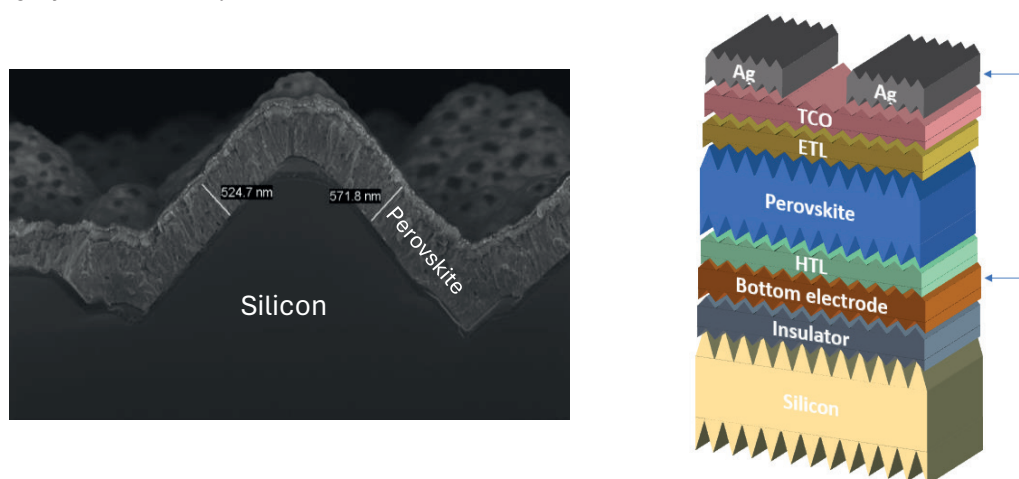


Figure 1.- Device a.) Cross-section SEM b.) layout used in this study.

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Stability of HTLs in co-evaporated perovskite solar cells with substrate configuration

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Perovskite solar cells (PSCs) in substrate configuration manufactured by co-evaporation present numerous advantages. Firstly, due to this fabrication method, uniform and thickness controlled films can be obtained over large areas, with great control of the environment and growth rate, adaptable to a wide range of substrates while minimizing material wastage. Secondly, employing this configuration expands the possibility of using different substrates, such as flexible films, and applying them to both single-junction and tandem solar cells, as it allows the incorporation of metal gridlines as a top electrode, minimizing resistivity losses. All of this enables the production of high-quality and high-performance solar cells, as well as facilitating large-scale manufacturing and application on flexible and multi-junction substrates.^[1]

One of the main challenges in these devices is their long-term stability under light and heat exposure, hence the need to study the influence of various hole transport layers (HTLs) on PSCs devices and their stability.

In this study, poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine (PTAA), N₄,N₄,N₄'',N₄''-tetra([1,1'-biphenyl]-4-yl)-[1,1':4',1''-terphenyl]-4,4''-diamine (TaTm), 2-(3,6-dimethoxy-9H-carbazol-9-yl)ethyl]phosphonic acid (MeO-2PACz), and 2-(3,6-Dibromo-9H-carbazol-9-yl)ethyl]phosphonic acid (Br-2PACz) are compared as potential HTLs due to their different properties. PTAA is a polymeric semiconductor with the characteristic of being electron-rich, facilitating hole transport and blocking electron penetration. Its excellent optical transparency in the visible range allows its use in semi-transparent or bifacial cells, besides showing high mechanical tolerance, making it suitable for flexible applications.^[2] TaTm is a small molecular weight arylamino molecule representative of molecules that are used as hole transport layers in the Organic Light-Emitting Diodes (OLED) industry due to its long lifespan. And finally, we have MeO-2PACz and Br-2PACz, which belong to the self-assembled monolayers (SAMs), which are being widely used lately due to their several advantages such as low cost, negligible optical and electrical losses in devices as well as their uniform coating for large-area substrates. MeO-2PACz has been extensively studied for its ease of processing, intrinsic scalability and absence of dopants, giving good results in terms of stability and efficiency. That is why it has also been compared with Br-2PACz because of its similar properties.^[3]

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Novel donor-acceptor dyads based on 30- π electron expanded hemiporphyrazines

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Within the world of porphyrinoids, the design of their expanded analogues appears very appealing from a functional and applicability viewpoint, since their core-modified conformation provides them unique photophysical and topological properties, which are inaccessible with respect to their non-expanded congeners. In addition, they possess a richer coordination chemistry with the ability to accommodate not only one but various cations of different size and nature in their coordination cavities and/or act as anions receptors, thus making them of particular interest. In contrast to the rich synthetic chemistry of expanded porphyrins (ExPor), relatively well developed to date,^[1] that of expanded porphyrazine analogues (ExHpz) remains, however, very scarce and still challenging.^[2,3] Although aromaticity tends to be an attractive feature of ExPors, it has to be noticed that in the case of expanded ExHpzs there is no diatropic ring current, which makes this family of macrocycles peculiar. As rare examples, our research group has previously reported the synthesis and characterization of several trithia-dodecaazahexaphyrins, which have been prepared by a [3+3] cross-condensation between a phthalonitrile derivative and 2,5-diaminothiadiaazole.^[2] Their structure consists of three units of isoindoline connected to each other *via* aza-bridges to three alternating thiadiazol moieties. However, all the reported examples of ExHpzs so far have been limited exclusively to symmetrically substituted ones (A_3 -type), with A being the isoindoline units peripherally functionalized with none ($R = H$) or solubilizing groups ($R = tBu, SR, OR, OAr$).

In this context, we have successfully prepared for the first time a novel non-symmetrical A_2B -type ExHpz analogue, peripherally substituted with two tBu groups (A) and one hydroxymethyl functional group (B) at the isoindoline positions. The two tBu groups aim to give solubility to the macrocycle while the alcohol functionality will allow us to combine several acceptors with it (including ferrocene, fullerene and pentacene derivatives) to prepare unprecedented donor-acceptor dyads and study their photophysical properties. In particular, it would be of great interest to unravel the energy/electron transfer process that would occur in these systems. Moreover, this novel ExHpz presents optical features that make it a potentially good candidate to be combined with pentacenes for singlet fission applications since it displays absorption bands that complement the absorption of pentacenes and overlap its emission.

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Defective nanographenes: synthesis and electron-transport properties at the single-molecule scale

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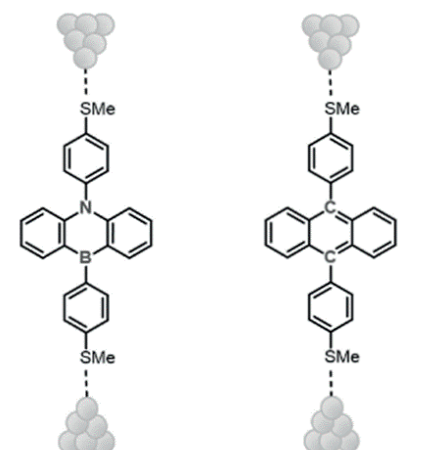
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Structural defects can induce significant alterations in the physical properties of graphene. Understanding the relationship between different types of defects and the changes promoted in the properties would make possible to find new and unexpected applications for defective graphene, exploiting the potential of this material.



The image shows two chemical structures side-by-side. The left structure is labeled 'BN doped π-skeleton' and features a central boron atom (B) bonded to two nitrogen atoms (N) in a six-membered ring, with two phenyl rings attached to the nitrogens. The right structure is labeled 'all carbon π-skeleton' and features a central carbon atom (C) bonded to two carbon atoms (C) in a six-membered ring, with two phenyl rings attached to the carbons. Both structures have a methylsulfanyl (SMe) group attached to the phenyl rings, and dashed lines indicate connections to a surface represented by a cluster of grey spheres.

In this work, we have used organic synthesis for preparing small graphene-like molecules presenting structural defects in a controlled manner. In particular, we have focused on two kind of defects: i) 7- membered rings, which take the molecule out of the plane and promote a negative curvature,¹ and ii) B-N (boracine) substitution, which gives rise to isolectronic structures with the non-substituted ones.² The electron-transport properties of these molecules have been studied by means of scanning tunnelling microscopy break-junction (STM-BJ) technique, which allows the evaluation of their electrical behaviour at the single-molecule scale.³ The results obtained for the defect-containing molecules⁴ have been compared with those obtained for their corresponding defective-free analogues. Additionally, theoretical calculations have been carried out in order to give a deeper understanding of the electron transport through these systems.

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La_{2-x}Ca_xSc_{1-y}Mg_yNbO_{7-δ}: Proton-conducting Ceramic Materials for Proton Ceramic Fuel Cells

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Solid oxide fuel cells (SOFC) are interesting energy conversion electrochemical devices, and an important support for the transition to a carbon-free future. In proton ceramic fuel cells (PCFC) the ceramic electrolyte transport protons from the anode to the cathode. The protons with low mass and high mobility allow the operation window to shift down to 350-600°C [1]. The most studied proton conducting electrolytes are

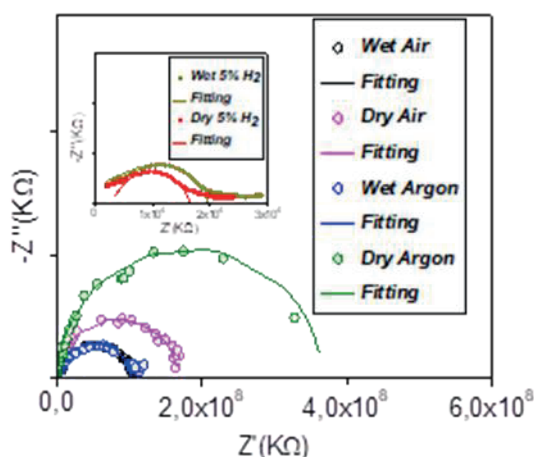


Fig. 1 Nyquist diagram of the impedance measurements at 550°C in dry and wet atmospheres of air, argon and 5% H₂ in argon.

perovskite-type oxides based on cerate or zirconate such as BaCeO₃, BaZrO₃ doped with rare-earth elements [2]. This work focuses on the development of new proton conducting ceramic materials that can be used as electrolyte [3] in PCFCs, decreasing the operating temperature compared to SOFCs, and improving the chemical and thermal stability. The La_{2-x}Ca_xSc_{1-y}Mg_yNbO_{7-δ} system, where x=0.00; 0.025; 0.05; 0.075 and 0.1; and y=0.00; 0.02; 0.05 and 0.1, was prepared by freeze-drying method, and structurally and morphologically

characterised by XRD and SEM. The ionic/electronic transport properties were determined by electrochemical impedance spectroscopy (EIS) [4], in the temperature range of 900-350°C, and in the presence of several dry and wet gases (Air, Argon, 5% H₂ in Argon). We have confirmed that this family of materials exhibits proton conductivity (Fig.1), which can be explained in terms of the Grotthuss mechanism.

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Chemical modification of 7,6-SWCNTs by Pd-porphyrin derivatives through different covalent approaches

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In recent years there has been a growing interest in carbon nanotubes, especially due to their superior mechanical, thermal, electronic, optical, and chemical properties. [1] The covalent modification of the carbon nanotubes (CNTs) onto their walls allows the improvement of the electronic properties and solubility of the materials to make them more useful for applications in the field of optoelectronics, such as photovoltaic devices. The covalent methods involve anchoring the moieties through the generation of new bonds [2] that usually lead to the saturation of the double bonds, causing the degradation of the sp^2 network responsible for the superior electronic properties and high electrical conductivity. [3] [4] In this work, we have used (7,6)-enriched SWCNTs for the development of CNT-based hybrid materials covalently functionalized with Pd-porphyrin derivatives bearing electron-rich triphenylamine groups at the meso- position, which may stabilize the porphyrin radical cation in the charge separation state favoring electron transfer process. [1] In this study, we have compared two covalent strategies, concretely functionalization via aryl diazonium salts, [5] and [2+1] cycloaddition through nitrene intermediates. [3]. Subsequently, we have characterized both nanohybrids using spectroscopic and thermogravimetric techniques. These characterization methods are crucial for assessing the structural integrity and composition of the developed materials. Additionally, we have analyzed the electronic and optical properties of the final materials, since understanding the conductive behavior is vital for evaluating the potential applications of these hybrid materials in optoelectronic devices.

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Impact of Pseudohalide Substitution on the Electrochemical and Magnetic Behavior of α Cobalt-Based Layered Hydroxide Materials

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Layered hydroxides (LHs) are two-dimensional (2D) materials based on earth-abundant elements that have shown interest in several fields such as catalysis, photochemistry, electrochemistry, polymerization, magnetization, biomedical science, and environmental application.[1] Recently, layered hydroxides have garnered significant attention for their exploration in electrochemistry and magnetism thanks to their good electrochemical behavior, chemical versatility, electrochemical stability, and low cost.[2] Herein, the epoxide route is utilized to obtain a pure α phase (simonkolleite-like structure) with flower-like morphology, distinguished by a covalent bond between the hydroxylated layer and the anion.

One of the major drawbacks of these materials is their low electrical conductivity, which represents a limitation in optimizing the electrochemical performance.[1] Among the different approaches to overcome this issue, we are intensively working on the modulation of the electronic properties of LHs. Indeed, we have recently demonstrated that the electrical properties can be modulated by halide substitution, where the band gap can be reduced by ligand-to-metal charge transfer.[3] Considering these previous results, we decided to investigate the pseudohalide influence on the electrochemical and magnetic properties of the Co-based α -layered hydroxide.

Our work initially centered on optimizing the synthesis by determining if the pseudohalide could drive the synthesis to attain the desired pure α phase. Regarding the magnetic properties, these phases behave similarly to the hydroxides reported in the literature, exhibiting magnetic ordering below 50K. All display a ferromagnetic predominance due to a positive Curie-Weiss temperature. Regarding magnetism, we observe a slight difference in temperature orders (T_B , T_M) depending on the pseudohalide. All exhibit characteristics of hard magnets. Exploring the electrochemical properties of the compounds on carbon paper in alkaline media shows that the α -Co-SCN phase performs better in redox measurements. The enhanced redox activity is interesting since it increases the conversion of Co^{2+} to Co^{3+} , making it more effective for the Oxygen Evolution Reaction (OER). This suggests that this material could be promising for energy systems, whose charge-exchange ability determines capacity.[4]

In view of this result, further studies will focus on optimizing an energy storage device employing pseudohalide-modified Co-LH as an electrode and electrocatalysis for OER.

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Twisted magnetic multilayers of CrSBr

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Two-dimensional van der Waals semiconductor CrSBr is a well-established candidate for the study of low-dimensional physics such as magneto-electronic coupling [1]. Recently a new type of the heterostructure of CrSBr was demonstrated, where two ferromagnetic layers were twisted by 90° forming a highly anisotropic multilayer device, and unintuitive step-like switching of the magnetoresistance (MR) has been observed [2]. Here we discuss possible mechanisms that can result in the step-like MR switching in such heterostructure as well as in similar twisted multilayer systems.

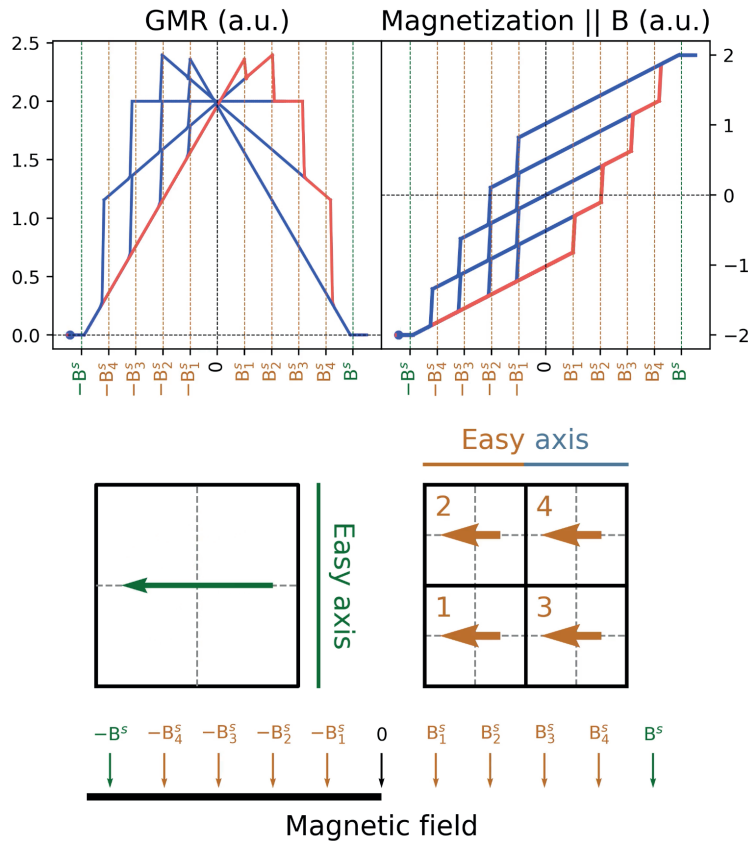


Figure 1. Domain switching mechanism of the step-like magnetization and magnetoresistance step-like behaviour in the orthogonally twisted bilayer of semiconductor CrSBr upon the magnetic field sweeps in the in-plane direction of the easy axis of one of the layers.

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Exploring the interaction and reactivity in graphene-antimonene heterostructures

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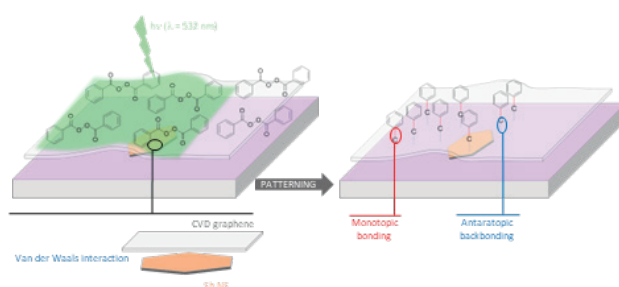
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The growing field of two-dimensional (2D) materials has recently witnessed the emergence of heterostructures formed by various multielemental 2D materials,[1] however experimental studies combining monoelemental layered materials remain relatively unexplored. In this regard, graphene is probably the most studied 2D building block and its reactivity is well established in the literature. On the contrary, the use of antimonene in these hybrid heterostructures has been barely studied. Nevertheless, antimonene is particularly interesting because of its pronounced interlayer interactions, inasmuch its atomic orbitals between individual layers contribute to a strong covalent character, surpassing the typical van der Waals (vdW) interaction.[2]

In this study, we present the chemical fabrication and characterization of a heterostructure formed by graphene and hexagonal antimonene. The interaction between these 2D materials is thoroughly examined through Raman spectroscopy and first-principles calculations, revealing that can be considered as a van der Waals heterostructure. Furthermore, we have explored the influence of the antimonene 2D material on the reactivity of graphene by studying the laser-induced covalent functionalization of the graphene surface, Scheme 1. Our findings indicate distinct degrees of functionalization based on the underlying material, being SiO₂ more reactive than antimonene, opening the door for the development of controlled patterning in devices based on these heterostructures. This research provides valuable insights into the antimonene-graphene interactions and their impact on the chemical reactivity during graphene covalent functionalization.



Scheme 1: Van der Waals heterostructure preparation based on hexagonal Sb and graphene, and its subsequent patterning through functionalization with benzyl substituents.

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Synthesis of graphene-layer double hydroxide hybrids for catalytic applications

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Nanomaterials, thanks to their unique elemental, size and morphological dependents properties, have generated significant interest in various fields of research and technology, such as optoelectronics, energy storage, and nanomedicine, among others. In this frame, the combination of two-dimensional (2D) materials with molecular or other nanomaterials compounds have demonstrated a promising pathway to enhance and tailor their properties for diverse applications, such as light-responsive materials and catalyst to mention few [1-2]. This study explores the potential of 2D-material hybrid heterostructures, specifically focusing on the combination of nickel-iron layered double hydroxides (NiFe-LDH) and graphene. NiFe-LDHs exhibit interesting electrochemical properties in electrocatalytic reactions like the Oxygen Evolution Reaction (OER), but face challenges in electrical conductivity, whereas graphene has exceptional conductivity and mechanical strength [3-5]. By combining these materials, synergistic effects can be achieved, potentially surpassing the limitations of individual components.

Herein, we present a novel approach to improve the electrocatalytic properties of NiFe-LDH for OER by synthesizing graphene-NiFe-LDH (G@LDH) 2D heterostructures. Two synthetic approaches were investigated to prepare G@LDH hybrids, yielding covalent and supramolecular hybrids [6]. Their structural and electrochemical properties were extensively characterized using microscopy, spectroscopic and analytical techniques. This work sheds light on the potential of graphene hybrid materials to boost the performance of LDH electrocatalytic hydrogen production.

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Magnetoelectric effect on Van der Waals heterostructures

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During the last years a whole field covering the exceptional and unique physical properties of two-dimensional layered materials have been developed. Some of the interaction and cooperative phenomena that come to play within those van de Waals heterostructures still need more exploration. Multiferroicity is one of them. Including the possibility of having the presence of two hysteretic orders in the same material to the 2D field unlocks novel potential application and vdW multiferroic heterostructures giving experimental support to fundamental mechanisms of the magnetoelectric coupling.

For that purpose, a proper characterization of the layered materials of interest will be done before their integration in the magnetoelectric heterostructure by combining electrical and magneto-optical measurements (MOKE). We will be focusing on few-layer CuInP_2S_6 , known to exhibit room-temperature ferroelectricity with out-of-plane polarization [1], and the CrI_3 , member of one of the first families of 2D magnets (insulating chromium trihalides CrX_3) which has been proved to be an Ising ferromagnet with out-of-plane spin orientation. [2]

An adapted set-up suitable for air sensitive materials that allow fabrication and transfer techniques in an inert atmosphere will allow us to explore some of the known characteristics of vdW materials: proximity and coupling effects, facility to transfer few-layer crystals on top of another and high susceptibility to gate voltages to tune their properties; giving us the possibility to explore the magnetoelectric effect through the fabrication of vertical van der Waals heterostructures by deterministically stacking a 2D ferromagnet (CrI_3) on top of a ferroelectric layer (CuInP_2S_6).

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Hyperspectral Microscopy for the study of layer dependent optical properties of different two dimensional materials.

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The implementation of the intrinsic magnetism, seen in 2D materials, into magneto-optic devices has been of great interest since its discovery in 2017. However, in order to integrate these magnetic materials into modern devices, the fundamental magnetic and optical properties must be further investigated to provide a better understanding. CrI₃ has shown great potential; with magnetism down to the monolayer, displaying a still unexplained phase transition from intrinsic antiferromagnetism in the few-layer to a ferromagnetic in the bulk.

Previous studies [2] have demonstrated that using Hyperspectral wide-field imaging for CrI₃, a non-monotonic thickness dependence of the complex optical dielectric function is present, which reveals three distinct thickness layer regimes: the Few layer (ranging from the monolayer to 13 atomic layers), the Multilayer (ranging from 13 layers to 100 layers) and the Bulk (beginning at 100 layers). The observed layer dependent optical properties and different thickness regimes seen are interesting, as they could provide important insight into the magnetic phase transitions seen in CrI₃.

This project seeks to explore the presence of these different thickness regimes in different two-dimensional materials (such as VI₃ and CrBr₃) using Optical Microscopy for the identification of regions of atomically thin flakes with varying layer thicknesses, Atomic Force Microscopy for layer height measurements and Hyperspectral imaging to demonstrate the change of the peak position as a function of the number of layers, showcasing whether the different thickness regimes are present in the sample in Transmission and Reflection wide-field hyperspectral measurements setups. Hyperspectral imaging provides a simple and non-destructive method to obtain a single shot of the light intensity coming from tens of crystals with different thicknesses, from which statistics can be obtained for analysis of the optical properties in the different regimes, providing insight into the different materials.

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Biaxial Strain of Single-Layer WS₂ Over a Wide Range of Temperature

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The micro-mechanical exfoliation of graphene in 2004 rekindled interest in two-dimensional (2D) materials. Among recently discovered 2D materials, single-layer transition metal dichalcogenides (TMDCs) are direct band gap semiconductors in its 2H structure, with band gap energies in the visible range. The strong interaction between electrons and holes is enhanced in the single-layer limit, resulting in their optical properties to be dominated by exciton dynamics [1]. Moreover, their high tunability and remarkable flexibility makes them ideal candidates for its implementation in flexible optoelectronics and allows a precise tuning of their properties via strain-engineering [2] [3].

In this study we present how the optical properties of single-layer semiconductor WS₂ can be tuned by biaxial strain induced by the controlled heating or cooling of samples deposited on thermoplastics substrates over a wide range of temperatures. Specifically, the effect of strain is tracked in the energy shift in the differential reflectance resonances associated to exciton formation. Firstly, we demonstrate excellent strain transfer both for tensile and compressive strain induced by heating up or cooling down, respectively, a single-layer WS₂ on a polycarbonate substrate. Additionally, we achieve a 0.5% compressive strain at room temperature. Subsequent cooling down to 4K results in an unprecedented degree of biaxial compressive strain by this method, up to ~ 1.6%, reflected in an energy shift of excitonic resonances by about 200 meV. Comparison of experimental and theoretical energy shifts with temperature suggests temperature-dependent gauge factors for large temperature ranges, likely due to the temperature dependence of the Young's modulus of polycarbonate.

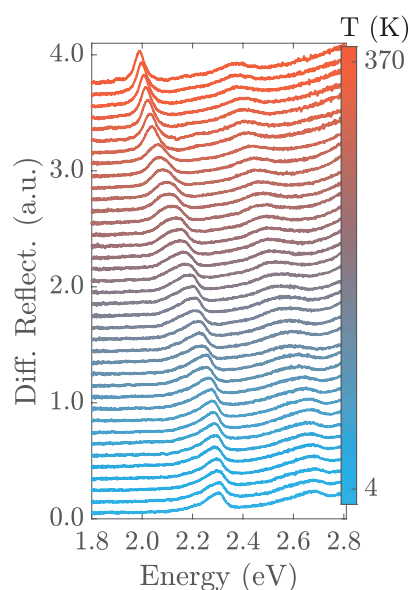


Figure 1: Differential reflectance spectra for single-layer WS₂ on a polycarbonate substrate for different temperatures.

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Growth and characterization of Ni-Fe ultra thin films on different buffer layers

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Magnetic thin films research is a field of outstanding importance in order to unravel some of the macroscopic magnetic properties (like the magnetization vector, different types of magnetic order, magnetic anisotropy, ordering temperatures) by studying the 'building blocks' at the micro and nano scale [1]. In addition, magnetic thin films are found in a wide variety of nowadays applications (data storage, spintronic devices) as well as in fields where there were not used some years ago, as a platform for biological applications and chemical sensors [2].

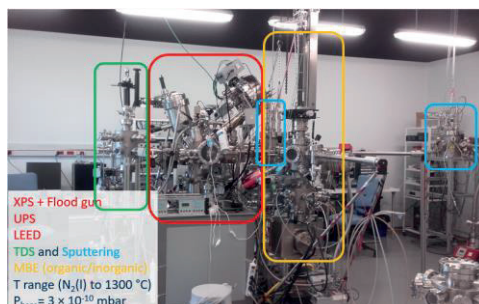


Figure 1: Epitaxial Growth laboratory at Imdea Nanociencia

The systems based on Fe and Ni are the focus of many research groups because it is possible to obtain a broad range of different behaviours by tuning the growth parameters [3-5]. In addition, Ni and Fe are not expensive and are some of the most abundant elements on Earth, which makes them good candidates for being used in common applications. In this work, we are going to study the chemical, structural, magnetic and morphological properties of thin films based on Ni and Fe and how those properties change with the use of different buffer layers. For that purpose, the films are going to be grown in Ultra High Vacuum conditions (see figure 1) and characterized with surface science techniques (*in situ* and *ex situ*).

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Improved strain engineering of atomically thin MoS_2 by polymer encapsulation

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Controlling the band structure through strain engineering is an exciting avenue for tailoring optoelectronic properties of materials at the nanoscale [1]. However, in the case of 2D materials, weak van der Waals interactions can cause severe slippage between the material and substrate, dominating the bending or stretching processes and leading to inefficient strain transfer. Encapsulation of 2D materials is a promising technique to reduce this slippage, as well as to improve the transferable strain [2]. This approach shows increased strain transfer in many cases, although it can be difficult to accomplish for some encapsulating layers or materials [3]. In this work we report a comparative statistical study of the strain transfer modulation of MoS_2 flakes on polypropylene substrates, which have been encapsulated with three different solution-based polymers: polycarbonate (PC), poly(methyl methacrylate) (PMMA) and poly(vinyl formal) (Formvar). The flakes have been covered following a simple and cost-effective technique, in which the polymers in solution are spin-coated on the 2D material. Through micro-reflectance spectroscopy, we have observed a remarkable increase in strain gauge factors, which have been obtained by direct bending of the substrate, as well as by changing its temperature. In the first case, uniaxial strain is achieved, while in the second case biaxial strain is achieved due to the much higher thermal expansion coefficient of the polypropylene substrate compared to the MoS_2 flakes. The gauge factors seen for non-encapsulated monolayer and bilayer MoS_2 through uniaxial mechanical strain are ~ 30 meV/%, while the ones achieved under the same conditions with PMMA or Formvar encapsulation lie around ~ 50 meV/%. Maximum transferable strain before slippage also increased with encapsulation, achieving best results for Formvar and PMMA. An improve in the lifetime of MoS_2 -based devices has also been observed. Finally, devices with Formvar encapsulation showed better photoresponse than their unencapsulated counterparts, as well as reduced dark current.

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