Book of Abstracts

Gandia
Valencia
Spain
2026

ESMolNa European School on Molecular Nanoscience

ESAM European School on Advanced Materials

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ESMolNa European School on Molecular Nanoscience

ESAM European School on Advanced Materials

W2dm Workshop on 2D Materials

	Sunday 17th	Monday 18th	Tuesday 19th	Wednesday 20th	Thursday 21st	Friday 22nd	
9:00-9:30		T Rojo	K Kanoda	R Oda	N Pascual		9:00-9:30
9:30-10:00						Brainstorming session:	9:30-10:00
10:00-10:30		M Giménez	L Bogani	R Matheu	S Mañas		10:00-10:30
10:30-11:00		MC Ruiz	J Arbiol	A Abhervé	A Forment		10:30-11:00
11:00-11:30		*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*	11:00-11:30
11:30-12:00		MA Herrero	O Céspedes	E Ortí	M Shatruk	Trends & perspectives in 2D Materials	11:30-12:00
12:00-12:30		E Pérez	D Zueco	E Ruiz			12:00-12:30
12:30-13:00		F Zamora	E Cánovas	L Escalera	S Barja		12:30-13:00
13:00-13:30	*LUNCH*						13:00-13:30
13:30-14:00		*LUNCH*	*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		C Herrmann	N Avarvari	J Puigmartí	H Van der Zant		16:30-17:00
17:00-17:30	*Welcome*						17:00-17:30
17:30-18:00		J Otón	J Barrio	MA Piqueras	Oral Comm.		17:30-18:00
18:00-18:30	N Martín	*Coffee break*	*Coffee break*	*Coffee break*	*Coffee break*		18:00-18:30
18:30-19:00		Oral Comm. & Flash presentations	Oral Comm. & Flash presentations	Oral Comm. & Flash presentations	Oral Comm. & Flash presentations		18:30-19:00
19:00-19:30							19:00-19:30
19:30-20:00	*Welcome cocktail*						19:30-20:00
20:00-20:30					*Closing & awards*		20:00-20:30
20:00-22:30	*DINNER*	*DINNER*	*DINNER*	*DINNER*	*DINNER & music*		20:00-22:30

Buffet restaurant is open for lunch from 13:00 to 15:30 and for dinner from 20:00 to 22:30

19th European School on Molecular Nanoscience- ESMoLNa2026
3rd European School on Advanced Materials- ESAM2026
12th Workshop n 2D Materials- W2DM2026

Gandia (Valencia, Spain) May 17th to 22nd, 2026

DETAILED PROGRAM

	SUNDAY 17th - ESMoLNa & ESAM	
13:00	*Lunch*	
16:00	*Registration*	
17:00	Miralles CORONADO- ICMol- U. València (ES)	*Welcome/Introduction to Molecular Nanoscience & Advanced Materials*
18:00	**Nazario MARTÍN- U. Complutense Madrid (ES)**	***Hacking Carbon Architectures: The Rise of Molecular Nanographenes***
19:30	*Reception Cocktail*	
20:30	*Dinner*	
	MONDAY 18th - ESMoLNa & ESAM	
9:00	**Teófilo ROJO- U. Basque Country-EHU (ES)**	***Challenges and perspective in Materials for Energy Storage and Conversion Systems***
10:00	María GIMÉNEZ LÓPEZ- CIQUS/U. Santiago Compostela (ES)	*Electrocatalysts Materials for Sustainable Energy Conversion*
10:30	Mª Carmen RUIZ DELGADO- U. Málaga (ES)	*Bridging Experiment and Theory: Unveiling Optical and Electronic Properties in Organic Materials*
11:00	*Coffee break*	
11:30	Mª Antonia HERRERO- U. Castilla-La Mancha (ES)	*Carbon nanomateriales as versatile platform*
12:00	Emilio PÉREZ- IMDEA Nanoscience (ES)	*Chirality in mechanically interlocked derivatives of carbon nanotubes*
12:30	Félix ZAMORA- UAM- IMDEA Nanoscience (ES)	*Processable Imine-Based COFs: From Molecular Design to Gels, Aerogels, Membranes, and 3D Printing*
13:30	*Lunch*	
16:30	**Carmen HERRMANN- U. Hamburg (DE)**	***First-principles and atomistic models for molecular electronics and spintronics***
17:30	Joaquín OTÓN- ALBA (ES)	*Multimodal Characterization of Advanced High-Strength Steels by X-ray & Electron Techniques*
18:00	*Coffee break*	
18:30	Alba ROMÁN FLORES- ICMol- U. València (ES)	*UIO-66 as platform for in situ encapsulation of nucleic acids and gene delivery*
6 mins Oral Comm	Alejandra SILVA MAYO- ICMol- U. València (ES)	*Interface and Architecture Optimization in PbPc-based Organic Photodetectors*
	Bogusława SMYKLA- Jagiellonian U. (PL)	*Anionic dithiolate-Au(I) complexes for the construction of luminescent heterometallic coordination assemblies*
	Julia REQUENA- ICMol- U. València (ES)	*Photochemical and Photophysical Properties of Carbon Nano-Onions Towards Combined Phototherapy Applications*
	Maja ROMANOWSKA- Jagiellonian U. (PL)	*Theoretical description of samarium(III) complexes: versatile simulation of optical and magnetic properties*
	Piotr GAS- Jagiellonian U. (PL)	*Photoluminescent micellar water sensor candidates based on block copolymer incorporating cyanido rhenium(V) complexes*
	Saskia MERZ CHULBI- Dept Química Inorg-anica- U. València (ES)	*Tailoring 1D Anilato-Based Coordination Polymers: Synthesis, Structural Studies, and Selective Sensing of Volatile Organic Compounds (VOCs)*
	Alberto MARTÍNEZ GÓMEZ- ICMol- U. València (ES)	*Multifunctional cascade enzyme nanoplatform for enhanced tumour starvation under hypoxic conditions*

3 mins Flash Pres.	El Mahdi HAMZA- U. Barcelona (ES)	*Preparation of nanoengineered Prussian Blue for energy storage*
	Ismael CASCALES ÁLVAREZ- U. Autónoma Madrid (ES)	*Functionalization of 3D-printed resins using Covalent Organic Frameworks*
	Polina LENKOVA TOPALSKA- U. Castilla-La Mancha (ES)	*Photoactive peptides for the creation of dynamic supramolecular hydrogels*
	Sara JIMÉNEZ BUITRAGO- U. Castilla-La Mancha (ES)	*Characterization of controlled release capacity of spherical diaminotriazine hydrogels incorporating magnetite nanoparticles*
	Teresa SAUCEDO CUBERES- U. Autónoma Madrid (ES)	*Polymeric solid electrolytes*
	Álvaro GARCÍA VICENT- ICMol- U. València (ES)	*Optimization of biomolecule confinement within UiO-66 hybrid biocomposites*
	Carlos MARTINEZ MARTIN- ICMol- U. València (ES)	*Ti-based MOFs as Biomimetic Artificial Metalloproteases*
	Pedro MARTÍNEZ RAJOY- ICMol- U. València (ES)	*Synthesis of acylhydrazone MOFs*
20:30	*Dinner*	
	TUESDAY 19th - ESMoLNa & ESAM	
9:00	Kazushi KANODA- U. Tokio (JP)	***Quantum Criticality in Organic Conductors: Electrons at the Edge of Classical and Quantum Worlds***
10:00	Lapo BOGANI- U. Firenze/Oxford (IT/UK)	*Topological invariants and the reactivity of carbon lattices: the hidden quantum mechanical foundations of Clar's rules*
10:30	Jordi ARBIOL- ICREA & ICN2 (ES)	*In-situ STEM for Energy and Catalysis Nanomaterials*
11:00	*Coffee break*	
11:30	Oscar CÉSPEDES- U. Leeds (UK)	*Tuning spin physics with molecular interfaces*
12:00	David ZUECO- INMA-CSIC (ES)	*Cavity QED with van der Waals chiral magnon cavities*
12:30	Enrique CÁNOVAS- IMDEA Nanoscience (ES)	*Electrical Characterization of Metal Organic Frameworks by Time Resolved THz Spectroscopy*
13:30	*Lunch*	
16:30	Narcis AVARVARI- MOLTECH-Anjou, CNRS-U. Angers (FR)	***Chirality related properties in molecular materials***
17:30	Jesús BARRIO HERMIDA- Imperial College London (UK)	*Design of carbon-based electrocatalysts with zeolitic imidazole frameworks*
18:00	*Coffee break*	
18:30	Adrián SANCHIS PERUCHO- U. Santiago Compostela (ES)	*Tuning Spin-Crossover Behaviour for Pressure-Induced Thermal Effects*
	Annena JESUMAN- ICMol- U. València (ES)	*Ammonia Induced Framework Transformations and Spin-Crossover in Fe(II) Hofmann MOFs*
	Carlos QUESADA PÉREZ- U. Alicante (ES)	*Competing spin correlations and their spectra between magnetic molecules coupled to superconducting leads*
	Carmen ROSALES MARTÍNEZ- ICMol- U. València (ES)	*Defect Engineering in Multivariate Metal–Organic Frameworks toward versatile applications*
	Diego LÓPEZ ALCALÁ- ICMol- U. València (ES)	*Chemical Engineering of Altermagnetism in Metal-Organic Frameworks*
6 mins Oral Comm	Garoé MEDINA-AGUILAR- U. Santiago Compostela (ES)	*Pressure-Activated Spin Crossover in flexible metallomesogens*
	Hubert DZIEŁAK- Jagiellonian U. (PL)	*Multifunctional coordination polymer with azido-pentacyanidocobaltate(III) linkers: impact of solvent vapor sorption on SHG, luminescence, and magnetism*
	Jan SIERZEGA- Jagiellonian U. (PL)	*Multifunctional molecular materials based on lanthanide complexes with dithiocarbamate ligands*
	María TAMAYO- ICMol- U. València (ES)	*Ultrastable pyrazolate porphyrin metal-organic frameworks for gas adsorption*
	Maria Amparo LOPO MARCH- ICMol- U. València (ES)	*Functionalized Metal–Organic Frameworks for Imaging*
3 mins Flash Pres.	David VALCARRERAS SANLORENZO- ICMol- U. València (ES)	*[1.1.1]propellane electrophilic activation by alkylboronates: a route to complex cyclobutanes*
	Hanane EL MANSOUR EL JASTIMI- ICMol- U. València (ES)	*Synthesis and characterization of novel spin crossover and single-molecule magnet complexes*
	Higinio MAQUEDA MÁRQUEZ- ICMol- U. València (ES)	*Reversible I_2 Uptake as a Strategy to Enhance Spin-Crossover Hysteresis in a Fe(II) Hofmann-Type MOF*

	Ramón RODRÍGUEZ MINIÑO- CIQUS - USC (ES)	*Towards Anthraquinone-Phosphonate Metal-Organic Frameworks*
20:30	*Dinner*	
	WEDNESDAY 20th - ESMoLNa & ESAM	
9:00	Reiko ODA- U. Bordeaux-CNRS (FR)	***Mesoscopic and hierarchical « chiral » objects to measure chirality***
10:00	Roc MATHEU- U. Barcelona (ES)	*Towards solid-solid phase change materials (PCMs) with high latent heat and thermal conductivity*
10:30	Alexandre ABHERVÉ- MOLTECH-Anjou, CNRS-U. Angers (FR)	*Chiral Halide Perovskites: Influence of Crystal Symmetry on Spin and Light Polarization*
11:00	*Coffee break*	
11:30	Enrique ORTÍ- ICMol- U. València (ES)	*Charge transport in organic semiconductors for perovskite solar cells*
12:00	Eliseo RUIZ- U. Barcelona (ES)	*Room-Temperature Single-Molecule Electronics: From Molecules to Supramolecular Entities*
12:30	Luis ESCALERA MORENO- TU. Hamburg (DE)	*Classical and Quantum Simulation of Materials for Quantum Technologies*
13:30	*Lunch*	
16:30	Josep PUIGMARTÍ- ICREA/U. Barcelona (ES)	***Unlocking materials innovation with microfluidic technologies***
17:30	Miguel Ángel PIQUERAS- OESIA (ES)	
18:00	*Coffee break*	
18:30	Ana PUCHADES ORTIZ- ICMol- U. València (ES)	*Sequential Vacuum Deposition of Cs/Cl-Alloyed FAPbI3 Perovskite Absorbers*
	Andrés MARTÍNEZ GARCÍA- U. Alicante (ES)	*Mechanosensitivity in dithia-helicenes through thermopower and conductance*
	Carsen Alise CARTLEDGE- ICMol- U. València (ES)	*Substrate Temperature Effects in Vacuum-Deposited Narrow Bandgap Perovskite Solar Cells Featuring In Situ Photoluminescence Monitoring*
	Guillem PELLICER- U. Alicante (ES)	*Quantum Transport Measurements in Single-Molecule Glycerol Junctions: A Machine Learning Analysis*
6 mins Oral Comm	Inma GOMAR-FERNÁNDEZ- ICMol- U. València (ES)	*Large Area Close-Space Sublimation Enables Efficient and Stable Perovskite Solar Cells*
	Lennart VAN DEN HENGEL- ICMol- U. València (ES)	*Evaporator design to tackle organic deposition speed bottle neck for Perovskite PV towards industrialization.*
	Michael MUSIOŁ- Jagiellonian U. (PL)	*Conductivity and Magnetization Switching in Ni-Fe Cyanido-Bridged Coordination Polymer Through H3O+/NH4+ Exchange*
	Moisés Gilberto ZARZOZA MEDINA- U. Castilla-La Mancha (ES)	*Magnetic, hydrogen-sensing, (Fe)Pd alloy nanoparticles and their oxidation to a Pd-FeOx core-shell structure*
	Austin Brooks WARWICK- U. Valladolid (ES)	*Green-Synthesized AuNPs from Grape Extracts: Extract-Dependent Effects on Nanoparticle Size and Sensor Performance*
	Carla BESELER LEÓN- U Politècnica València & U. València (ES)	*Synergistic Antimicrobial Activity of Natural Peptide-Functionalized Mesoporous Silica Nanoparticles Loaded with Essential Oil Components*
	Francisco Javier CARRASCO TORRES- ICMUV- U. València (ES)	*Lead Halide Perovskite Nanocomposites for Down-Conversion LEDs*
3 mins Flash Pres.	Julieta VELASCO MARTÍNEZ-PARDO- U. Autónoma Madrid (ES)	*Label free magnetic nanoparticles as dual nanothermometers/nanoheaters: from CoFe2O4 to Synomag*
	Lucía MARTÍNEZ MOYA- ICMol- U. València (ES)	*Close-Space Sublimation for Perovskite/Silicon Tandem Solar Cells*
	Manuel REGUILÓN MONCIÓN- ICMol- U. València (ES)	*Dry-Processed Wide-Bandgap Perovskite Solar Cells*
	Raquel HERNÁNDEZ BENÍTEZ- ICMol- U. València (ES)	*Design and Enantioselective Performance of a Copper-Based Metal-Organic Framework*
20:30	*Dinner*	
	THURSDAY 21st - ESMoLNa & ESAM & W2DM	
9:00	Nacho PASCUAL- CIC NanoGUNE (ES)	***Magnetic nanographenes on superconductors: topology, edge spins, and YSR states***

10:00	Samuel MAÑAS- ICMol- U. València (ES)	*Quantum sensing with 2D materials: imaging magnetic waves*
10:30	Alicia FORMENT- ICMol- U. València (ES)	*Molecular tools for 2D materials*
11:00	*Coffee break*	
11:30	Michael SHATRUK- Florida State U. (USA)	***Principles of Materials Design for Efficient Spin-State Swithiching in Ultrathin Layers***
12:15	Sara BARJA- U. Basque Country-EHU (ES)	***From Surface Science to Electrochemistry: Model Systems for Interface and Reaction Studies***
13:30	*Lunch*	
16:30	Herre VAN DER ZANT- T.U. Delft (NL)	***Spin-Hall effect in magnetic graphene***
17:30 6 mins Oral Comm	Calisa Carolina DA SILVA DIAS DE OLIVEIRA- ICMol- U. València (ES)	*Curie Temperature Enhancement and Modified Magnetic Universality Class in 2D $CrCl_3$ via epitaxial growth*
	Daniela Alejandra CÉSPEDES LLANOS- ICMol- U. València (ES)	*Solution-processed asymmetric functionalization of POM-sensitized MoS2 for enhanced HER*
	Federico JUAREZ DOMINGUEZ- ICMol- U. València (ES)	*Electrochemistry in NiFe-LDH*
	Filippo MIONE- ICMol- U. València (ES)	*Strongly bound excitons in the layered material BiI3: a thickness and temperature dependent study*
18:00	*Coffee break*	
18:30 6 mins Oral Comm	Giuseppe DI MAIO- U. Calabria (IT)	*2D Gold Nanocubes Monolayers: A Multifunctional Plasmonic Architecture for Electronics and Sensing*
	Luuk MURIS- ICMol- U. València (ES)	*Systematic Raman study of β-Ni(OH)2: Disorder and influence of cations*
	Marc LÓPEZ MOLLÁ- ICMol- U. València (ES)	*Covalent Surface Functionalization of 2D-Bismuthene Nanosheets*
	Patricia FERRER ALCARAZ- U. Alicante (ES)	*Correlation between growth conditions and superconducting performance in e-beam deposited Nb thin films*
	Paula TORRES GARCÍA- INAMOL. UCLM (ES)	*Unconventional physical behaviors of highly corrugated superconducting niobium thin films*
	Youssra DIOUANE- ICMol- U. València (ES)	*Stepwise Compositional Design of High-Entropy NiFe-LDHs for Enhanced Oxygen Evolution Reaction Performance*
3 mins Flash Pres.	Ainhoa CANO- IMDEA Nanociencia (ES)	*Designing amphiphilic DNA nanostructures through synthetic control*
	Haritz MENTASTE RUIZ- ICMol- U. València (ES)	*Modulating WSe2 photoluminescence through ferroelectric polarization coupling in a van der Waals heterostructure*
	Laura GONZÁLEZ CERVERA- ICMol- U. València (ES)	*Implementation of 2D Materials in Memristive Materials for Neuromorphic Computing*
	Luis MARCO SABATER- ICMol- U. València (ES)	*Design of small molecules for the degradation of 3D DNA structures*
	Natalia CASTRO REINA- ICMol- U. València (ES)	*Surface Engineering of MoS_2 with Polyoxometalates toward Improved HER Performance*
19:45	Closing and GENAM-RSEQ Awards to best Flash Presentation or Oral Communication	
20:30	*Dinner & music*	
	FRIDAY 22nd - W2DM	
9:30	Brainstorming session: Trends and perspectives in 2D Materials	
11:00	*Coffee break*	
11:30	Brainstorming session: Trends and perspectives in 2D Materials	
13:00	*Lunch*	

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Abstracts index in alphabetical order

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Synergistic Antimicrobial Activity of Natural Peptide-Functionalized Mesoporous Silica Nanoparticles Loaded with Essential Oil Components

Carla BESELER-LEÓN[1], Miguel REYES-TORRES[1], Ramón MARTÍNEZ-MÁÑEZ[1,2,3,4,5], María Dolores MARCOS[1,2,3,5], Andrea BERNARDOS[1,2,3,5].

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[2]*CIBER de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN).*
[3]*Unidad Mixta UPV-CIPF de Investigación en Mecanismos de Enfermedades y Nanomedicina, Universitat Politècnica de València, Centro de Investigación Príncipe Felipe. C/ Eduardo Primo Yúfera 3. 46012, Valencia, Spain.*
[4]*Unidad Mixta de Investigación en Nanomedicina y Sensores. Universitat Politècnica de València, Instituto de Investigación Sanitaria La Fe (IIS La Fe), Valencia, Spain.*
[5]*Departamento de Química, Universitat Politècnica de València, Valencia, Spain.*

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The emergence of multidrug-resistant pathogens, particularly **ESKAPE bacteria,** represents a major global concern, as commonly used antibiotics became ineffective, compromising the efficacy of treatments and increasing the prevalence of infections [1]. This issue has led to the requirement for effective and innovative antimicrobial therapies. In this context, the use of **delivery systems**, especially mesoporous silica nanomaterials, elicited significant attention due to the ability to encapsulate compounds of interest, and functionalized with molecular gates, preventing cargo leakage, providing them stability and **controlled release** in presence of an external stimulus [2].

In this study, **mesoporous silica nanoparticles (MSNs)** were loaded with an **essential oil component (EOC).** The surface of the nanoparticles was anchored with negatively charged carboxylate groups, onto which the cationic antimicrobial peptide (AMP), **ε-poly lysine**, was grafted electrostatically. This peptide acts as a **molecular gate** that triggers the release of the EOC in acidic pH condition, produced by bacterial metabolism. The system was characterized by general techniques, including powder X-ray diffraction (PXRD), scanning transmission electron microscopy coupled with Energy Dispersive X-Ray Spectroscopy (STEM-EDX), zeta potential or thermogravimetric analysis (TGA), confirming that the nanodevice has been correctly synthesized.

To evaluate antimicrobial and synergistic effects, a clinically relevant pathogen, such as *Staphylococcus aureus*, has been used. The antimicrobial activity of the system was assessed through microbiological assays such as minimal inhibitory concentration (MIC) and dose response curves, confirming inhibitory properties at **low doses**, and a bactericidal behavior since it has achieved the **eradication** of the bacterial cells. Fractional inhibitory concentration index (FICI) was calculated between the free compounds in the nanoparticle to assess the presence of **synergistic interactions**, obtaining a potent synergy among different cargos and the molecular gate. These findings highlight the potential of MSN-delivery systems as a promising approach to **combat antibiotic-resistant pathogens.**

References

[1] Ho, C.S. et al, Antimicrobial resistance: a concise update. *Lancet Microbe* **2025**, 6 (1), 100947.
[2] Bernardos, A. et al, Mesoporous Silica-Based Materials with Bactericidal Properties. *Small* **2019**, 15 (24), 1900669.

DESIGNING AMPHIPHILIC DNA NANOSTRUCTURES THROUGH SYNTHETIC CONTROL

Ainhoa Cano-Vázquez[1], Mario Martinez[1], Álvaro Somoza[1]

[1]*IMDEA Nanociencia, Nanotechnology for Health, Calle Faraday 9, 28049, Madrid*

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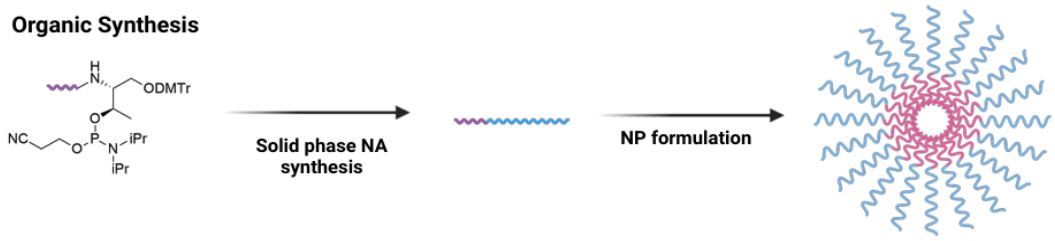
Amphiphilic Nucleic Acids (ANAs) represent a powerful class of customizable biomaterials that combine the specificity of DNA recognition with the self-assembly of lipids. The resulting morphology is primarily determined by the hydrophilic/hydrophobic balance, where the length and unsaturation of the lipid tails dictate the packing within the core. By precisely controlling the synthetic design and environmental factors, such as pH and ionic strength, it is possible to modulate electrostatic interactions and induce hierarchical transitions, shifting from discrete spherical micelles to higher-order structures like nanorods or nanofibers [1].

The synthesis of these ANAs relies on solid-phase synthesis (SPS) and phosphoramidite chemistry, which allow the site-specific integration of modifications into DNA strands. By employing custom-made lipid-phosphoramidite building blocks, it is possible to introduce hydrophobicity at precise positions along the oligonucleotide sequence. This approach offers unparalleled control over the spatial distribution of lipids, ensuring high coupling efficiency and the ability to scale the production of complex amphiphilic structures [2] [3].

In this context, we propose the modification, via organic synthesis, of nucleotide analogs with long-chain fatty acids of varying degrees of unsaturation, which can be employed to modulate the amphiphilicity of nucleic acids. These derivatives are transformed into their corresponding phosphoramidites and are then utilized in SPS to obtain the desired oligonucleotides. After that, their purification is carried out via Polyacrylamide Gel Electrophoresis (PAGE) to ensure high structural homogeneity. Further characterization will be fulfilled using Transmission Electron Microscopy (TEM) to evaluate the morphological impact of different lipid tails and environmental conditions on the formation of higher-order nanostructures. These findings are expected to enhance our capability to engineer highly customizable DNA-based nanotechnology."



Scheme 1. Synthesis of DNA-based amphiphilic nanostructures using solid-phase synthesis and phosphoramidite chemistry

References

[1] Zhang, Y., et al. Hierarchical self-assembly of cholesterol-DNA nanorods. *Bioconjugate chemistry* **2019,** *30*(7), 1845-1849

[2] Anaya, M., et al. Tunable hydrophobicity in DNA micelles: design, synthesis, and characterization of a new family of DNA amphiphiles. *Chemistry–A European Journal* **2010**, *16*(43), 12852-12859.

[3] Gubu, A., et al. Nucleic acid amphiphiles: Synthesis, properties, and applications. *Molecular Therapy Nucleic Acids* **2023,** *33*, 144-163.

Lead Halide Perovskite Nanocomposites for Down-Conversion LEDs

Fco. Javier CARRASCO[1], Mario PRIETO[1], Rafael ABARGUES[1]

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Perovskite:$M(OAc)_2$ nanocomposites (M = Ni or Mg) are excellent candidates for down-conversion LEDs. We report a double-composite architecture embedding these emitters within a poly-2-ethyl-2-oxazoline (PEOX) matrix. This structure increases the film thickness to ~1330 nm, doubling photoluminescence (PL) intensity, and demonstrates high versatility across diverse A-site cations (MA, FA, Cs, and mixtures). Beyond traditional moisture-driven growth [1, 2], we introduce an *in-situ* crystallization method mediated by polar solvents in the vapor phase. Crucially, the PEOX matrix is highly compatible with these vapors, thereby accelerating crystallization and yielding superior optical properties. This vapor route successfully crystallizes MA- and FA-based systems, notably enabling the growth of highly emissive $FAPbBr_3$-$Ni(OAc)_2$ composites, whereas these nanocrystals completely fail to form under standard humidity. Reaching near 100% photoluminescence quantum yields (PLQY) and outstanding photostability under continuous blue LED stress, this synergistic approach provides a robust and reproducible platform for perovskite optoelectronics.

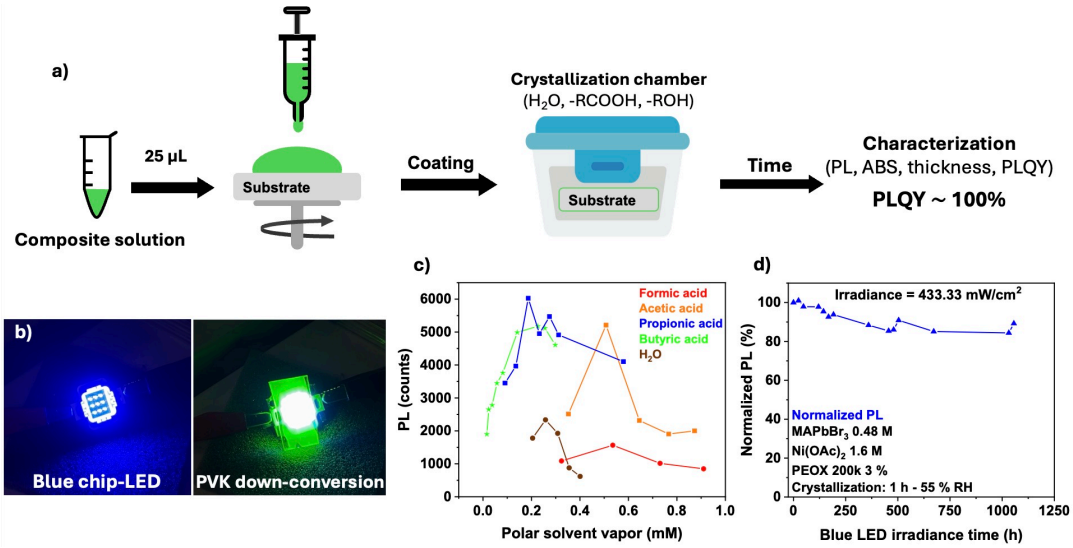

Figure 1. (a) Schematic representation of the vapor-assisted *in-situ* crystallization method using a hermetic chamber. (b) Visual demonstration of the green down-conversion emission from the $MAPbBr_3$-$Ni(OAc)_2$ nanocomposite film under blue LED excitation. (c) PL intensity kinetics as a function of exposure time to different polar solvent vapors. (d) Long-term photostability study of the optimized films under continuous blue LED stress.

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Substrate Temperature Effects in Vacuum-Deposited Narrow Bandgap Perovskite Solar Cells Featuring In-Situ Photoluminescence Monitoring

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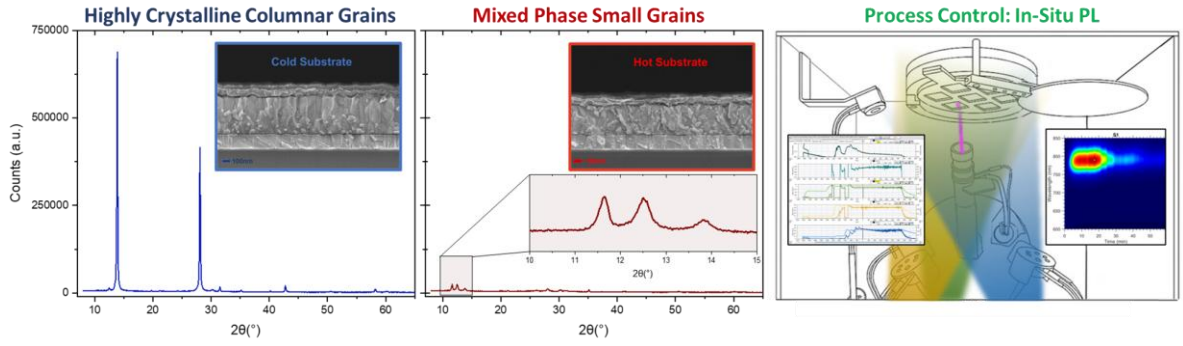
Perovskites have emerged as a leading material of interest in the development of next-generation photovoltaic technologies, offering tunable bandgaps and low-temperature processing. Although the active layer is typically fabricated using solution-based methods, dry vacuum-based techniques have emerged as an appealing alternative with the potential of large-area manufacturing. Interestingly, the relationship between deposition parameters and device properties proves complex due to competing factors in the film [1]. In this work, we investigate how substrate temperatures from −20°C to 70°C influence the growth and device-relevant properties of co-evaporated formamidinium methylammonium lead iodide (FAMAPI) films through the use of various standard characterization techniques as well as in-situ photoluminescence measurements which offer a novel, real-time indication of film quality during deposition.

A systematic assessment of structural, optical, and compositional characteristics across the stated temperature range was carried out using ex-situ techniques such as X-ray diffraction, electron microscopy, and optical spectroscopy. Furthermore, in-situ photoluminescence monitoring was implemented during the FAMAPI deposition as a complementary diagnostic tool that is sensitive to process-dependent changes which determine the quality of the final film.

Overall, this work provides early insight into the temperature-dependent crystallization pathways of evaporated FAMAPI perovskites and establishes a framework for correlating in-situ photoluminescence with device-relevant film quality. These findings highlight substrate temperature as a powerful lever for tuning vacuum-processed narrow-bandgap perovskites and point toward new strategies for optimizing their performance in photovoltaic applications.



Microstructure evolution under varying substrate temperatures and real-time monitoring via in-situ photoluminescence during deposition provides a powerful lever for tuning vacuum processed perovskites.

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Functionalization of 3D-Printed Resins using Covalent Organic Frameworks

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Covalent organic frameworks (COFs) are crystalline and porous materials synthesized by a bottom-up approach from molecular building blocks that are linked together by reversible covalent bonds. Their well-defined pore sizes, high surface area values and versatile functionalization make them ideal for multiple applications such as gas and energy storage, water treatment or catalysis. [1] To implement COFs, they need to be processed so that they can operate under real conditions, which usually involves designing systems capable of working under continuous flow. Hybrid catalytic systems based on coating MOFs onto 3D-printed resins were recently developed and successfully used for the cycloaddition of CO_2 to epoxide groups under flow conditions. [2] Based on these precedents, the aim of this work is to prepare COF coatings on 3D-printed resins and subsequently evaluate them as catalytic systems under operating conditions. Thus, imine-type COF coatings have been successfully prepared under mild conditions on resin substrates (Figure 1). These materials have been characterized by common techniques like FT-IR spectroscopy, powder X-ray diffraction and SEM microscopy among others. In situ introduction of Ru nanoparticles will enable the use of these devices as catalysts in hydrogenation reactions with good recovery and recyclability.

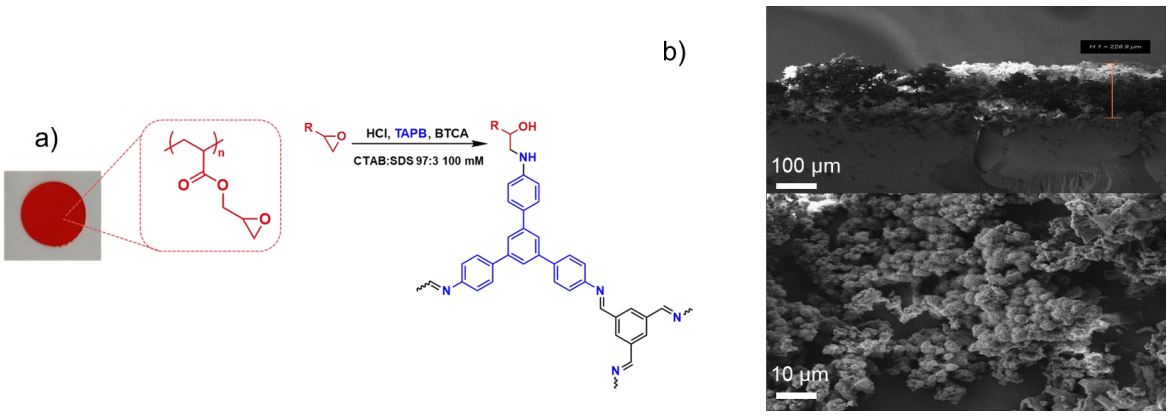

Figure 1: a) Chemical structure of a 3D-Printed polymeric resin and post functionalization reaction to produce a COF coating. b) SEM image of COF coating onto a 3D-printed resin.

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Surface Engineering of MoS_2 with Polyoxometalates Toward Hydrogen Evolution Reaction

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As the global transition toward a decarbonized hydrogen economy accelerates, the development of cost-effective and scalable catalysts for the hydrogen evolution reaction (HER) has become a priority. Replacing noble metal-based catalysts with earth-abundant materials is key to reducing the cost of green hydrogen production.[1]

In this context, molybdenum disulfide (MoS_2) has emerged as a compelling candidate, though its performance is limited by both a poor in-plane conductivity and the inert nature of its basal plane, being only active on the edges of the material.[2] Among the different strategies to boost the intrinsic HER activity of MoS_2, interface engineering with functional, redox-active molecules has emerged as a promising strategy.

In this context, we have employed polyoxometalates (POMs) as molecular counterparts. POMs possess exceptional redox versatility and unique physicochemical properties, including rapid multielectron transfer and stabilization of mixed-valence intermediates. When interfaced with solid substrates, POMs act as efficient electron–proton reservoirs, generating synergistic interfacial effects that enhance the activity and durability of the supporting material. POMs have also been widely explored as standalone HER catalysts,[3] which can further enhance the capabilities of the resulting 2D-based nanocomposites. However, despite the appealing physicochemical properties of POMs, their combination with MoS_2 remains largely unexplored.[4]

In this presentation, I will show our latest advances in the fabrication of POM/MoS_2 nanocomposites as a promising strategy to tune the HER properties of MoS_2.

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Solution-processed asymmetric functionalization of POM-sensitized MoS_2 for enhanced HER

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Polyoxometalates (POMs) are inorganic redox-active materials typically composed of early transition metals in high oxidation states connected through oxygen bridges. Their nanometric dimensions allow them to be regarded as a type of oxide-based quantum dots (QDs) with a very high surface to bulk ratio [1]. In parallel, two-dimensional (2D) materials exhibit pronounced electronic confinement and unique optical properties. In this context, MoS_2, one of the best-known members of the transition-metal dichalcogenide (TMDC) family, shows properties that are strongly dependent on the synthesis method and preparation conditions. [2].

Hybrid materials integrating both systems bridge their complementary structural and functional characteristics. MoS_2 provides an extensive accessible surface with catalytically active sites, particularly for the hydrogen evolution reaction (HER). POMs inherently enhance their electrocatalytic potential by offering abundant active sites that can act as redox active metal centers, while also providing high activity and selectivity for the formation of hierarchical structures and excellent performance in electrocatalytic processes [3].

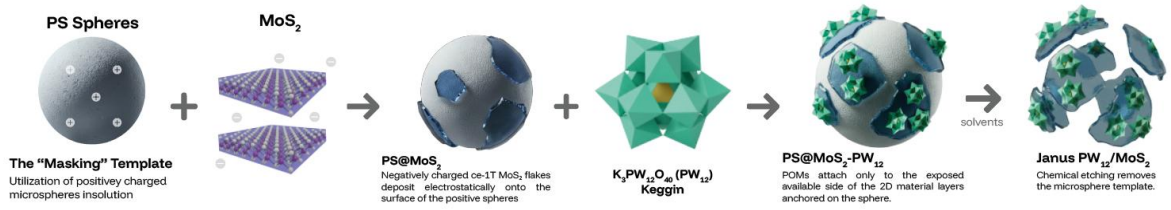

Figure 1. Schematic representation of liquid-phase asymmetric functionalization process.

Therefore, integrating POMs with 2D MoS_2 into hybrid heterostructures represents a promising strategy to enhance electrocatalytic performance. In this regard, the exploration of alternative assembly routes, such as asymmetric functionalization could increase the effective surface area and enable a controlled distribution of active sites. To achieve this, we employed a technique previously developed by some of us for the selective functionalization of 2D materials [4], using a sacrificial inert template to mask one face of the 2D sheet, leaving the other face available for chemical grafting. We present our preliminary results on the preparation of Janus-type POM/MoS_2 heterostructures and their characterization using microscopic and spectroscopic techniques to evaluate their chemical properties and catalytic potential.

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Curie Temperature Enhancement and Modified Universality Class in 2D $CrCl_3$ via Controlled Epitaxy.

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Low-dimensional (2D) van der Waals materials, in which magnetic order is present, have been an emerging area of fundamental and applied research [1,2]. Particularly, the CrX3 (X=Cl, Br, I) semiconductor class of van der Waals layered material presents layer-dependent magnetic properties when lowering dimensionality to a monolayer, and in particular distinct magnetic anisotropies: out-of-plane easy axis for CrBr3 and CrI3, and easy plane for CrCl3 [3].

In this context, this work will explore the tunability of the magnetic behavior of an already established 2D XY magnet, CrCl3, with a critical temperature of ~13K [4]. Herein, we produce a large-scale and high-quality monolayer (ML) of CrCl3 grown on two distinct surface structures: the SiC(0001) superstructure $6\sqrt{3}x6\sqrt{3}R30^\circ$ and Pristine(1x1) SiC(0001). This experiment was carried out fully in a UHV environment, from the growth via Molecular Beam Epitaxy to magnetic characterization using x-ray magnetic circular dichroism (XMCD) at ALBA Synchrotron.

We successfully demonstrated the growth of CrCl3 ML with distinct crystalline order, resulting in a significant change in magnetic behavior, such as enhancement of phase transition temperature up to 18K and magnetic moment in the order of 3.79 μB. These results reinforce how precise control of epitaxial growth can lead to substantial improvement of magnetic critical temperatures and changes in the magnetic universality class.

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2D Gold Nanocubes Monolayers: A Multifunctional Plasmonic Architecture for Electronics and Sensing

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Gold nanoparticles (AuNP) 2D monolayers are characterized by intense, isotropic, and in plane optical and electrical responses in a reduced thickness, which are noteworthy features for innovative nanomaterials development in electronics and sensing fields. [1] However, their realisation is very challenging due to the large number of parameters involved in the formation of ordered AuNP arrays, requiring a careful choice of the fabrication technique and building-blocks. Among the fabrication methodologies available, the most valuable is the self-assembling at immiscible solvents interfaces, which are ideal, defect-free surfaces minimizing process variables and enabling the creation of large, ordered monolayers. Furthermore, gold nanocubes (AuNC), with their planar facets and a strong plasmon field localized on their sharp edges, are ideal candidates as building blocks for 2D monolayers realization. [1,2]

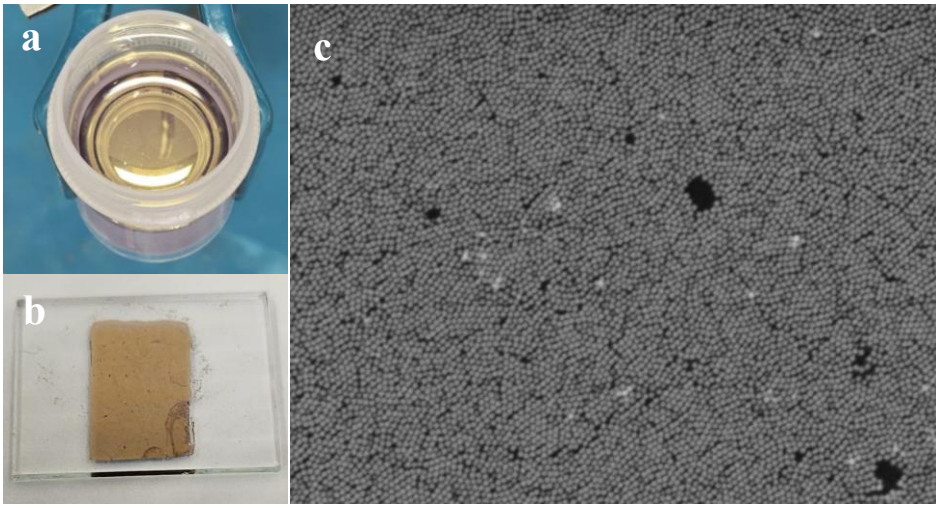

Figure 1. AuNC 2D monolayer at water-hexane interface (a), and deposited on ITO/Glass substrate (b, c).

In this work, an experimental procedure for the fabrication and optical, morphological and electrical characterization of large-scale AuNC 2D monolayers deposited on solid substrates (glass, ITO) was developed, including both the AuNC seed-mediated growth synthesis and interfacial self-assembling processes optimization. [3] The as-obtained AuNC 2D monolayers (see Figure 1) were employed both as metal-Enhanced Fluorescence platform as well as for the realization of hybrid biological-inorganic conductive substrates through the functionalization with dsDNA chains. [3,4]

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Stepwise Compositional Design of High-Entropy NiFe-LDHs for Enhanced Oxygen Evolution Reaction Performance

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The growing demand for sustainable energy technologies has intensified efforts to develop efficient electrocatalysts for water splitting. Alkaline water electrolysis is a promising strategy for green hydrogen production; however, its overall efficiency is limited by the sluggish kinetics of the oxygen evolution reaction (OER). Among the most active catalysts in alkaline media, NiFe layered double hydroxides (NiFe-LDHs) have attracted considerable attention due to their high intrinsic activity and tunable structure.[1,2] Recently, high-entropy layered double hydroxides (HE-LDHs), which incorporate five or more principal elements in near-equimolar ratios, have emerged as a promising class of materials, showing enhanced OER performance compared to conventional NiFe-LDH. The improved catalytic activity is often attributed to entropy-driven stabilization and the synergistic interactions between multiple transition metals within the LDH structure.[3-6]

In this work, we report the synthesis of HE-LDHs derived from the NiFe-LDH platform through a progressive compositional design strategy. Starting from the conventional system, additional transition metals are gradually incorporated into the layered structure, increasing the number of elements from binary compositions to multicomponent systems containing five, six, and seven metals. This stepwise approach allows us to systematically probe the influence of compositional complexity on the OER performance and to track the evolution of catalytic activity as the entropy of the system increases. Experimentally, a non-linear trend in OER activity is observed where catalytic performance initially decreases with the progressive addition of metals, reaching a minimum at four elements, before reversing to a clear enhancement as the number of elements increases from five to seven. Density functional theory (DFT) simulations reveal a similar trend, providing atomic-level insight into the electronic structure and adsorption energetics of key OER intermediates and supporting the role of multi-metal interactions in modulating catalytic performance.

Through combined experimental and computational analysis, this work advances understanding of structure-property relationships in high-entropy LDHs and opens a versatile playground for future studies aimed at enhancing their oxygen evolution performance.

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Multifunctional coordination polymer with azido-pentacyanidocobaltate(III) linkers: impact of solvent vapor sorption on SHG, luminescence, and magnetism

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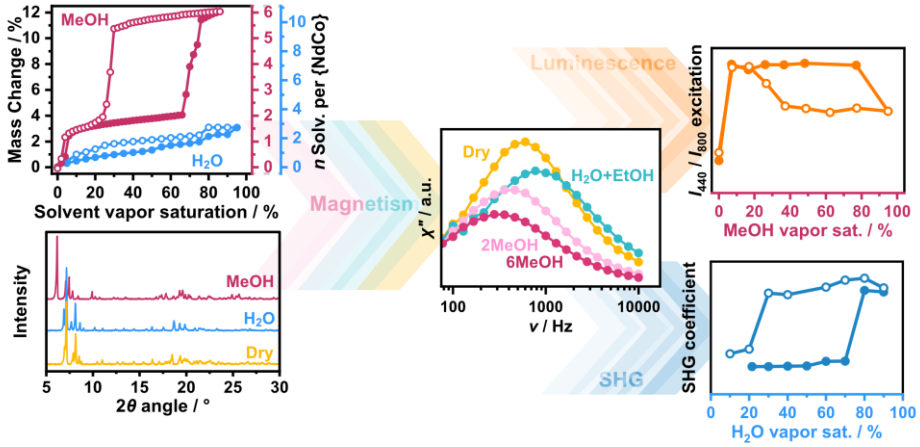
Lanthanide(III) (Ln) complexes have been recognized as a source of multifunctional magnetic materials [1]. The special interest is devoted to the interaction between the generated properties. In this regard, a considerable number of physical effects were combined in the Ln-based molecular materials, which include solvent vapor sorption linked with molecular nanomagnetism [2] or the latter combined with second harmonic generation (SHG) and luminescence [3]. Here, we present the pathway for merging the four mentioned functionalities. We combined a rarely explored azido-pentacyanido-cobaltate(III) ion, a novel metalloligand able to form π–π interactions and H-bonds, as well as coordinate to Ln ions [4], with NIR-emissive and magnetic Nd(III) complexes bearing diphenylphosphine ligands. The resulting Nd(III)–Co(III) coordination polymer exhibits relatively strong Nd(III)-centered emission with solvent (MeOH, EtOH, H_2O) vapor sorption. It crystallizes in a polar $P2_1$ space group, which allows for SHG to be observed, and the distinct magnetic anisotropy of Nd(III) leads to the slow relaxation of the magnetization. It was found that both MeOH and H_2O vapors significantly change the whole set of magnetic and optical characteristics, making this compound a unique stimuli-responsive multifunctional opto-magnetic molecular switch (see figure below).



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Synthesis and Characterization of Novel Spin-Crossover and Single-Molecule Magnet Complexes

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This study explores the magnetostructural correlations in two new neutral heteroleptic complexes synthesized using the doubly deprotonated 2,6-bis(3-(trifluoromethyl)-1H-1,2,4-triazol-5-yl)pyridine (H_2L) ligand in combination with the bis(pyrazolyl)pyridine (bpp) family of derivatives. The design of such heteroleptic systems follows established strategies for fine-tuning spin-crossover (SCO) properties through ligand substitution in iron(II) and combination with single-molecule magnet (SMMs) properties by introducing cobalt(II). The reaction with **Cobalt(II)** and **bpp** yielded two distinct crystalline phases of the [Co(bpp)L] complex. Static (DC) magnetic measurements confirm a pure octahedral Co(II) environment with a characteristic $\chi_M T$ value of approximately 2.7 $cm^3 \cdot K \cdot mol^{-1}$. Dynamic (AC) susceptibility studies, performed under an applied DC field of 1000 G reveal frequency-dependent signatures and prominent peaks in the out-of-phase (χ'') signal. These results, supported by narrow distribution parameters in the Cole-Cole plots, confirm SMM behavior. The isostructural character of one of these phase with the previously prepared iron(II) complex will enable preparation of iron(II)/cobalt(II) mixtures in the search of synergy between SCO and SMM properties. On the other hand, preparation of an iron(II) complex with L^{2-} and the fluorinated ligand **bppF$_2$** results in the [Fe(bppF$_2$)L] complex which displays an abrupt spin transition, suggesting high cooperativity within the crystal lattice facilitated by the fluorinated substituent. These findings demonstrate that subtle modifications in the ligand field and metal center can effectively toggle the system between bistable magnetic relaxation and abrupt spin-state switching, offering a promising platform for multi-functional molecular electronic devices.

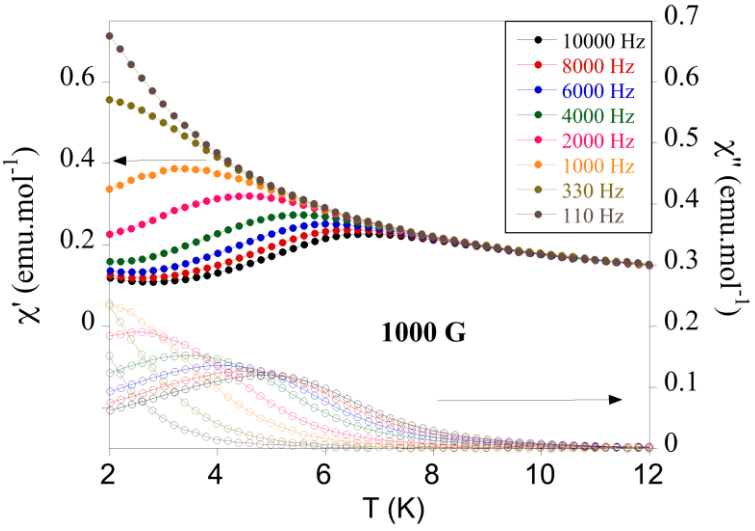

Figure 1. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') AC magnetic susceptibility for the heteroleptic Co(II) complex under a 1,000 G DC field. The frequency-dependent peaks in the χ'' signal indicate slow relaxation of the magnetization, characteristic of single-molecule magnet (SMM) behavior.

Correlation between growth conditions and superconducting performance in e-beam deposited Nb thin films

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Niobium thin films are widely used in superconducting devices; however, achieving bulk-like superconducting properties remains challenging when using electron-beam evaporation. In this work, we investigate the influence of key growth parameters on the superconducting properties of Nb thin films, including critical temperature (Tc), critical current (Ic), and critical magnetic field (Hc). We find that increasing both the deposition rate and the substrate temperature leads to a significant improvement in superconducting performance. This behaviour is attributed to enhanced adatom mobility and reduced incorporation of contaminants during growth, resulting in denser films with improved microstructural quality. Our results highlight the importance of jointly optimizing growth parameters to achieve high-quality Nb thin films by e-beam evaporation, providing practical guidelines for superconducting device fabrication.

Optimization of biomolecule confinement within UiO-66 hybrid biocomposties

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Metal-Organic Frameworks (MOFs) are hybrid porous materials that have recently emerged as highly versatile platforms for the encapsulation and protection of biomolecules due to their tunable porosity and structural robustness.[1] Despite first general, promising examples of hybrid nanostructures,[2,3] an optimal internal microenvironment that maximizes both framework stability and protein function under physiological conditions remains a significant challenge. Thus, it is essential to develop specific biomolecule-MOF hybrids with tailored chemical compositions for the desired biomolecules.

We propose the *in-situ* synthesis of zirconium-based MOF biocomposites, specifically UiO-66. This archetypal MOF has been recently obtained by some of us using synthetic conditions compatibles with bioentities.[4] Its modular chemical platform enables ligand functionalization, which results a very convenient strategy to rationally modulate the protein-MOF interface. By systematically incorporating functionalized organic linkers with varying electronic and steric profiles (e.g., -Br, $-CH_3$, $-NH_2$), we aim to fine-tune the hydrophobicity and local physicochemical properties of the cavities.

In this work, we will demonstrate that targeted ligand engineering approach in Zr-MOFs can effectively preserve the integrity of encapsulated biomacromolecules and enables the evaluation of their functional performance in *in vitro* cell culture systems, paving the way for advanced biotechnological applications in biocatalysis and targeted therapeutics.

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Photoluminescent micellar water sensor candidates based on block copolymer incorporating cyanido rhenium(V) complexes

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The construction of novel functional materials with increasing application potential stands out as one of the primary goals of today's materials science. Organic-inorganic hybrid materials are a particularly attractive research pathway, as combining building blocks of distinct natures often allows for broadening the possibilities offered by both of them separately. We explore this research direction by combining strongly photo-luminescent $[Re^{V}(CN)_4(N)]^{2-}$ (N^{3-} = nitrido ligand), which is a molecular functional unit that has previously exploited in the context of optical thermometry, order-disorder phase transitions and volatile organic compounds sensing,[1] with organic polystyrene-*block*-poly(4-vinylpyridines) (PS-*b*-P4VPs), which represent a well-studied class of amphiphilic block copolymers, known for their ability to self-assemble and act as templates for functional materials.[2] We have synthesized the composite materials and explored the features that they show, especially focusing on the micellar nanostructures formed in solution. The mentioned micelles have been found to allow for the emission of the Re(V) complex previously unobservable in solution, as well as to be extremely sensitive to the presence of water, which causes them to decompose. These factors allow for the construction of a water sensor with optical readout, based on the mechanism of luminescence quenching coupled with the composite micelle decomposition (Figure 1).

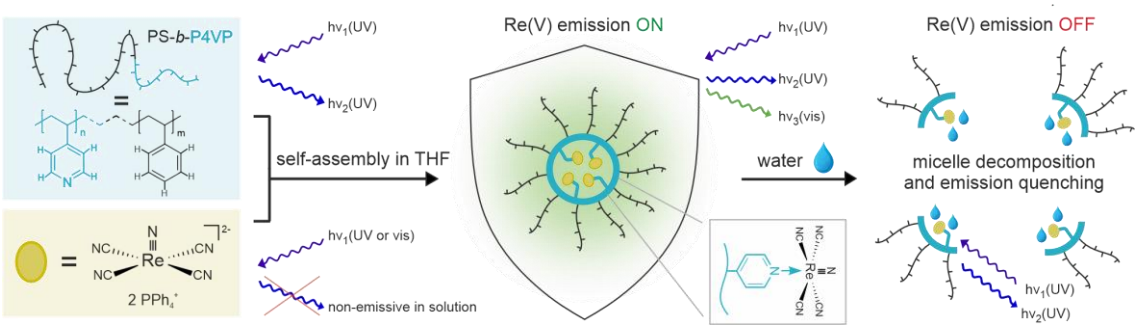

Figure 1. Representation of the basic principles of the reported work, including the emission turn-on and turn-off mechanism related to the composite micelle decomposition.

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Large Area Close-Space Sublimation Enables Efficient and Stable Perovskite Solar Cells

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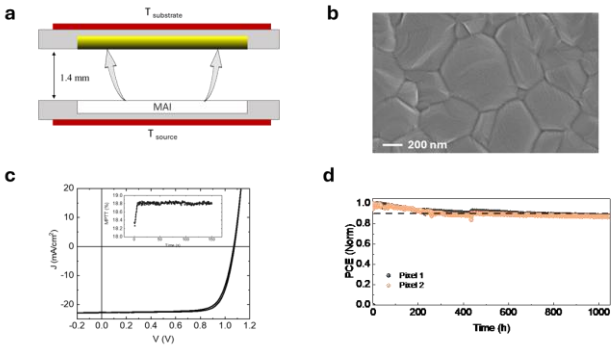
The rapid advancements in perovskite solar cells (PSCs) have positioned them as a leading candidate for next-generation photovoltaic technologies, driven by their remarkable efficiency[1] and versatility in fabrication methods. In this work, we present methylammonium lead iodide (MAPI) perovskite films deposited using a large area close-space sublimation (CSS) technique. [2] The process relies on a tempered methylammonium iodide (MAI) source with an active area of 96 cm², which ensures stability and reproducibility over a long number of cycles, simplifies handling, and reduces material consumption. The large-area CSS system enables the simultaneous conversion of multiple samples under moderate vacuum conditions (1 mbar), offering a scalable and straightforward alternative to other high-vacuum deposition techniques. The system allows for parallel deposition on six 3×3 cm² substrates, and its three-plate design—with independently heated top and bottom plates—providing precise temperature control during the conversion process. The resulting perovskite films exhibit large grains and uniform coverage, supporting efficient current collection even with relatively thin absorber layers. These CSS prepared films lead to solar cells with power conversion efficiency (PCE) of 18.8 %. The solar cells have extraordinary stability; they retain 90 % of their initial efficiency after operating for 1000 hours at their maximum power point at 75 ºC and 1 sun illumination. These results highlight the potential of the CSS method as a scalable, solvent-free, and reliable route for producing high-quality perovskite films and efficient solar cells.



a.Schematic of the CSS process b. top-view SEM image of the resulting perovskite film c. JV curve for the best pixel with stabilized power output measured for 100 s d. Normalized power output of the device during MPP tracking operation of two different pixels for 1000h.

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Implementation of 2D Materials in Memristive Materials for Neuromorphic Computing

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The exponential growth of AI and IoT technologies demands memory devices with superior speed and energy efficiency. However, conventional von Neumann architectures suffer from performance and power limitations due to the strict separation between processing and memory units.[1] Organic semiconductor-based memristors present a promising path forward: their resistance switching arises from ion migration within the active layer, emulating synaptic plasticity.[2] Nevertheless, ion-driven memristive responses typically exhibit volatile retention times (< 1 ms), impeding stable long-term operation. In this work, we present a strategy to enhance memory retention by integrating exfoliated two-dimensional (2D) materials, such as MoS_2, into a Super Yellow polymer matrix doped with triflate salts (XTriflate, X = Li, Na, K), Figure 1a. The 2D nanosheets provide additional anchoring sites and tailored diffusion pathways for mobile ions, facilitating tunable resistance states through controlled cation–2D material interactions, Figure 1b. Our approach offers a pathway toward organic memristors with improved stability and retention, advancing the development of energy-efficient neuromorphic hardware for next-generation computing.

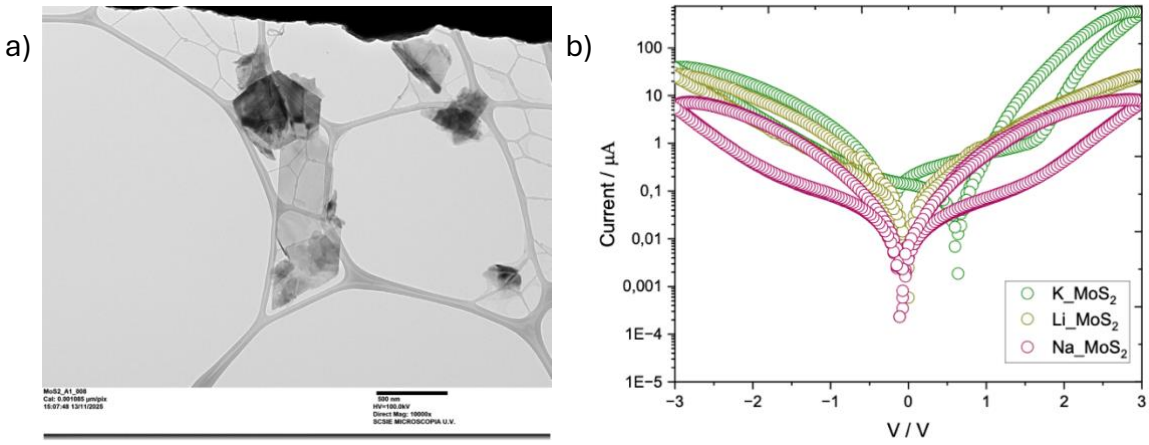

Fig. 1. a) MoS_2 tip sonication exfoliated flake by transmission electron microscope (TEM). b) Current/voltage measurement of the Super yellow MoS_2 with triflate salts (XTriflate, X = Li, Na, K).

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100-words summary

Preparation of nanoengineered Prussian Blue for energy storage

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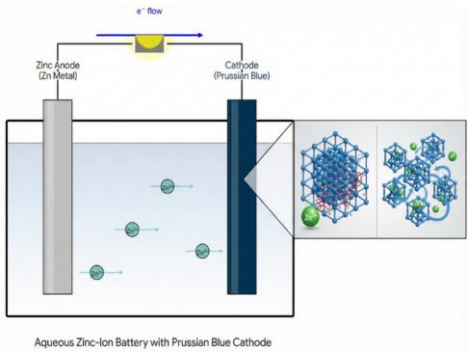
In the search for advanced materials for zinc-ion batteries (AZIBs), Prussian Blue (PB) has emerged as a high-potential candidate. The optimization of its electrochemical performance is intrinsically linked to the material's morphology; therefore, this research proposes reducing the particle size from the conventional micrometric scale (1-2 µm) toward a target nanometric range of 3-5 nm. The fundamental purpose of this dimensional transition is to minimize the diffusion length of Zn^{2+} cations within the PB crystal lattice, thereby facilitating more efficient charge-transfer kinetics during insertion and extraction processes (redox reactions).

To achieve this precise dimensional control, two chemical synthesis methodologies have been explored. The first involves the use of polyvinylpyrrolidone (PVP) as a capping and steric stabilizing agent. PVP encapsulates the primary crystallization nuclei, delimiting their growth and preventing agglomeration. Through this method, nanoparticles between 20 and 50 nm have been obtained, identifying the molar ratio between PVP and the precursors as the critical parameter. Currently, a 5:1 ratio is being utilized; observations indicate that higher polymer concentrations favor a decrease in particle diameter, showing potential for achieving even smaller dimensions.

Simultaneously, a microemulsion technique based on the surfactant sodium bis(2-ethylhexyl) sulfosuccinate (AOT) has been implemented. This system allows the chemical reaction to be confined within inverse micelles, which act as nanoreactors that mechanically restrict crystal growth. Through this approach, particles of approximately 10 nm have been synthesized, offering a promising route not only for size reduction but also for enhancing the crystallinity of the material—a determining factor for structural stability and the cycle life of the cathode.



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Design and Enantioselective Performance of a Copper-based Metal-Organic Framework

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The separation of enantiomers remains a fundamental challenge in the pharmaceutical industry, as different chiral forms of a drug can exhibit significantly different biological activities. Although high-performance liquid chromatography (HPLC) using polysaccharide-based chiral stationary phases, such as Lux Cellulose-3, remains the standard for enantiomeric resolution, the development of alternative porous materials with enhanced selectivity and tunability is highly desirable. In this context, metal-organic frameworks (MOFs) have emerged as promising candidates due to their structural versatility and the possibility of incorporating chiral functionalities directly into their frameworks [1,2]. Ibuprofen, widely administered as a racemic mixture, represents an attractive model compound for evaluating enantioselective separation strategies. We report the synthesis of a copper-based MOF functionalized with a chiral ligand derived from L-serine, designed for the enantioselective resolution of racemic ibuprofen. The chirality of the framework promotes stereoselective host-guest interactions within its porous structure, enabling differential adsorption of the enantiomers. The material was evaluated in a solid-phase extraction (SPE) configuration, and the enantiomeric composition of the eluates was analyzed by HPLC. The results reveal a preferential adsorption of the S-enantiomer, achieving an enantiomeric excess of 38%, demonstrating the potential of the MOF as a chiral porous material for enantioselective separations.

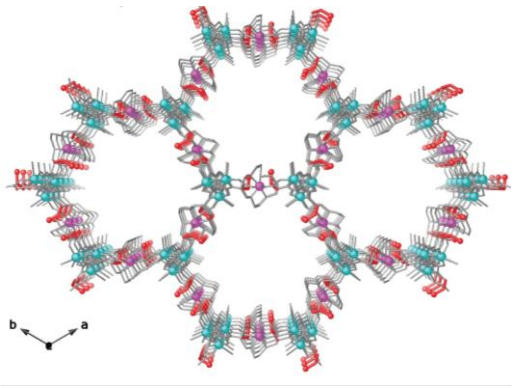

Figure 1. Molecular structure of the Copper-based Metal-Organic Framework

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"Ammonia Induced Framework Transformations and Spin-Crossover in Fe (II) Hofmann MOFs"

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Fe(II)-based metallorganic frameworks (MOFs) are particularly notable for their spin-crossover (SCO) behaviour, in which the electronic states of the metal centres respond to external stimuli such as temperature, pressure, light or analyte absorption. [1,2] This switching is accompanied by pronounced changes in magnetic, optical, and structural properties, making SCO systems a rich playground for investigating structure–property relationships. We explore $[Fe(pz)M(CN)_4]$ (M = Pd, Pt) frameworks, where incorporation of bifunctional ligands such as pyrazine (pz) links the 2D $\{Fe–[M(CN)_4]\}_\infty$ layers into robust 3D networks that enhance cooperative effects.[1] Exposure to ammonia (NH_3), a small, strongly coordinating Lewis's base, induces reversible clathrate formation while preserving the topology, yet dramatically shifts spin-transition temperatures by up to 150 K and partially stabilizes the high-spin state. They demonstrate that host–guest chemistry is a powerful lever to finely tune the structural, electronic, and magnetic properties of heterometallic Hofmann-type frameworks.

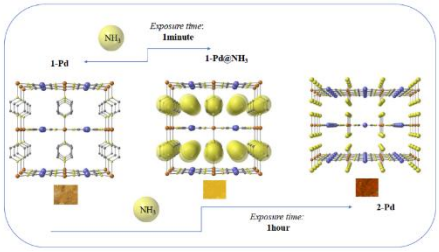

Figure- Pictorial description of ammonia absorption and coordination over a given time period

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Characterization of controlled release capacity of spherical diaminotriazine hydrogels incorporating magnetite nanoparticles

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The biological activity of a compound does not only depend on its chemical nature: administration and consequent absorption by the organism must be also considered. Macroscale drug delivery (MDD) devices enable spatiotemporal control over drug release [1]. In this context, hydrogels are three-dimensionally crosslinked polymeric networks capable of retaining large amounts of water within their structure. Their similarity to the extracellular matrix of soft tissues makes them ideal for MDD systems.

However, most bioactive compounds are poorly hydrophilic, complicating their encapsulation and later release from hydrogels. To address this, diaminotriazine-based networks are proposed, as they contain hydrophobic domains that interact with such species. In addition, magnetite nanoparticles will be incorporated into the matrix (Figure 1). By applying variable magnetic stimuli, drug release can thus be controlled [2].

The system will also exhibit a hollow, spherical geometry; as hydrogel gelation is light triggered, it is possible to 3D print the desired shape. The material aims to function as a cell culture scaffold that imitates ovarian architecture, while also allowing magnetic control over release of growth factors into the inner region, where immature oocytes will be cultured. This design will better mimic the 3D physiological conditions within the ovary, thus improving the efficiency of the *in vitro* maturation (IVM) of the gametes [3].

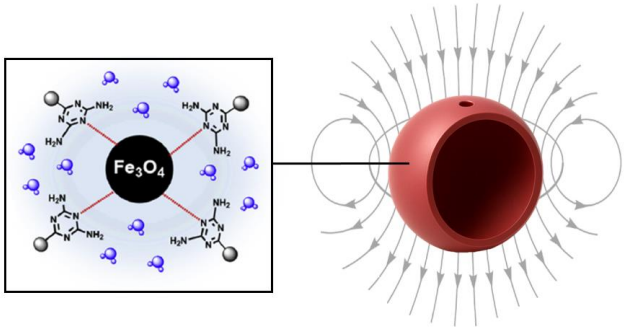

Figure 1. Magnetite nanoparticles embedded in the diaminotriazine-based hydrogel.

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Electrochemical behaviour of NiFe-LDH, kinetics and performance.

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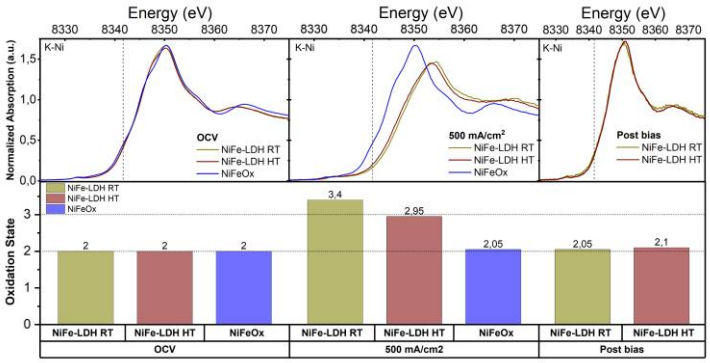
Efficient and scalable oxygen evolution reaction (OER) catalysts based on earth-abundant elements are essential for the commercial advancement of anion exchange membrane water electrolyzers (AEMWE). Among various candidates, NiFe layered double hydroxides (NiFe-LDHs) have emerged as the state-of-the-art non-PGM materials in alkaline media; however, their practical implementation is still challenged by unresolved questions regarding structural integrity and long-term operational stability[1]. In this work, we present a systematic electrochemical study of an epoxide-derived NiFe-LDHs previously developed by our group, which has demonstrated outstanding performance in preliminary assessments[2]. Here we focus on the potential correlation between redox reversibility and oxygen evolution performance relative to a conventional benchmark. Our findings suggest that catalytic efficiency may be linked to the material's ability to attain higher oxidation states and undergo reversible phase transitions[3]. By analysing the redox behaviour, we explore how the reversibility of the $Ni^{+2}/Ni^{+3}/^{+4}$ couple serves as a potential descriptor for the electrochemical behaviour and intrinsic activity of the LDH system. The epoxide-derived NiFe-LDH exhibits enhanced OER performance compared to the benchmark, while simultaneously displaying a more pronounced reversible electrochemical response. Complementary in situ Extended X-ray Absorption Fine Structure (EXAFS) measurements reveal that Ni in the LDH lattice can access oxidation states beyond Ni^{+3} under OER conditions. This highly dynamic redox behaviour coincides with the observed reversibility, suggesting a possible link between the accessibility of high-valent Ni states, electrochemical reversibility, and the overall durability of NiFe-LDH catalysts.



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Photoactive peptides for the creation of dynamic supramolecular hydrogels

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Inspired by biological systems that operate outside of thermodynamic equilibrium, the goal is to design adaptive "living" materials where the assembly and disassembly of nanostructures are reversibly controlled by light stimuli.[1] The primary objective is to design programmable, transient peptide materials that respond to external stimuli, specifically light, to govern structural reorganization without chemical fuels.

The research involves the design and synthesis of hydrophobic dipeptides made of leucine and phenylalanine (Leu-Phe) using solid-phase peptide synthesis (SPPS) with the Fmoc strategy.[2] These sequences will be functionalized with azobenzene units at various positions—the N-terminus, the peptide backbone, or side chains—to explore how their location influences photoactive behavior. Characterization will be conducted via NMR and LC-MS, while photoisomerization will be evaluated using UV-Vis spectroscopy under UV (365 nm) and visible (455 nm) irradiation. Furthermore, supramolecular self-assembly into fibrillar networks and hydrogel morphology will be analyzed using TEM, SEM and Raman.

The project aims to establish a clear correlation between azobenzene positioning, peptide sequence, and the ability to form reversible hydrogels. By determining mechanical properties and reversibility through rheology, this work will provide critical data for the rational design of photoactive materials. These advancements represent a significant step forward in non-equilibrium dynamic materials, with potential applications in soft robotics and controlled drug delivery.

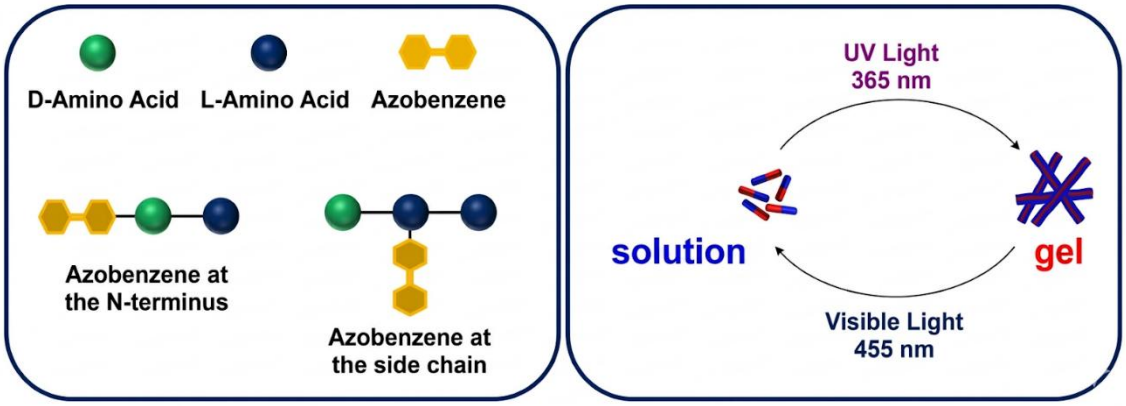

Figure 1. Schematic representation of the azobenzene-functionalized peptides designed, incorporating azobenzene at different positions along the peptide chain (left). Solution-to-gel (and viceversa) conversion cycle of the peptides through light irradiation at different wavelengths.

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Chemical Engineering of Altermagnetism in Metal-Organic Frameworks

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The recent identification of altermagnetism as a distinct magnetic phase has opened a new conceptual framework for spin-dependent phenomena beyond conventional ferro- and antiferromagnetism,[1] yet its realization has so far been largely restricted to a relatively narrow set of inorganic materials.[2] In contrast, molecular systems—and in particular metal–organic frameworks (MOFs)—provide an unexplored chemical space as a platform for emergent magnetic phenomena.[3] In these systems, magnetic order, exchange interactions and, crucially, symmetry can be precisely engineered. Here, we demonstrate that low-dimensional MOFs can host altermagnetic behavior, giving rise to spin-split electronic structures in the absence of net magnetization. In these systems, symmetry plays a central role in defining the emergence of altermagnetic states, highlighting how electronic structure can be controlled through chemical design.[4] Furthermore, we show that altermagnetism can be intrinsically coupled to spin crossover in MOFs, providing a route toward switchable altermagnetic materials. These results position MOFs as a promising and highly adaptable platform for extending altermagnetism into the realm of molecular magnetism and open new perspectives for the design of spintronic functionalities in chemically programmable materials.[5]

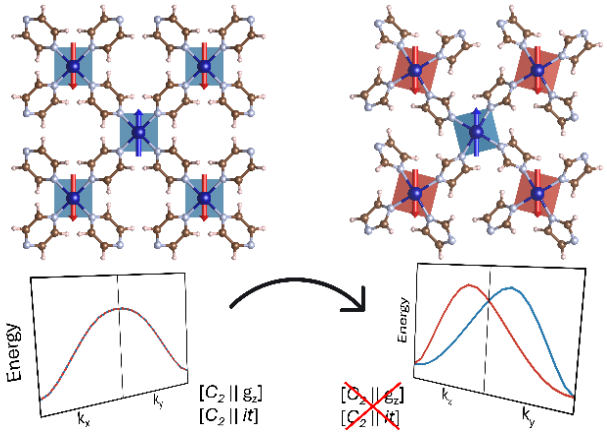

Figure 1. Chemical engineering of altermagnetism in a 2D MOF via symmetry breaking.

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Covalent Surface Functionalization of 2D-Bismuthene Nanosheets

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The growing interest in 2D pnictogens (P, As, Sb and Bi) for applications in catalysis and nanomedicine contrasts with the limited advances in their covalent chemistry. In particular, the covalent functionalization of bismuthene remains a major challenge due to its intrinsic structural and electronic features, which hinder controlled surface modification and the formation of stable functional derivatives. As a result, this field is still largely unexplored, with only a few studies and limited structural or chemical characterization available in the literature.[1,2,3]

This work presents a significant step forward by introducing a covalent anchoring strategy based on epoxide ring-opening reaction, enabling controlled surface decoration with reactive functional groups. The methodology is applied to nanosheets synthesized through two independent routes (colloidal and hydrothermal), allowing for the first direct comparison of how the material's origin and crystallinity influence its surface reactivity.[4] Using a comprehensive set of advanced spectroscopic and structural techniques, we elucidate the mechanisms governing the interaction at the bismuth interface, demonstrating that the metallic phase is preserved upon functionalization. Overall, this study provides new insights into the surface chemistry of bismuthene and establishes a foundation for the design of hybrid architectures and complex heterostructures with tailored properties.[5,6]

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Functionalized Metal–Organic Frameworks for Imaging

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Metal–organic frameworks (MOFs) constitute outstanding candidates as nanocarriers for medical imaging due to their unique properties, including ultra-high surface area, permanent porosity, multifunctionality and ease of chemical modification.[1] Post-synthetic surface functionalisation with ligands such as phosphate-functionalised methoxy polyethylene glycol (mPEG–PO_3) is a well-established strategy to improve colloidal stability and biocompatibility.[2]

In this work, PEGylation was first investigated to stabilize MOF nanoparticles under biological conditions. We combine this strategy with an alternative approach by surface functionalisation with oligonucleotide DNA sequences, creating a large set of nanoMOF nanoparticles designed to be more versatile and programmable. UiO-66 was selected as a model MOF system to study the effect of different surface functionalisation strategies on nanoparticle stability and functionality. The nanomaterials were synthesised *via* the solvothermal method, and their structure, size and morphology were confirmed by Powder X-ray Diffraction (PXRD), IR spectroscopy and TEM. Then, the colloidal stability of nanoMOFs was evaluated by monitoring the hydrodynamic size over time in different biological media using Dynamic Light Scattering (DLS). In addition, the degree of DNA functionalisation was quantified, allowing determination of the percentage of DNA successfully attached to the nanoparticle surface.

The incorporation of NaF, as an analogue of PET tracers, was investigated by ^{19}F NMR, demonstrating the ability of the nanoMOF nanoparticles to host fluoride species within their porosity. Finally, biological studies were performed in several cancer cell lines, including cell viability, zirconium accumulation and organelle localization. The developed systems exhibited good stability under biological conditions, successful DNA functionalisation, and the ability to incorporate NaF, highlighting their potential as multifunctional platforms for future imaging applications.

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Reversible I_2 Uptake as a Strategy to Enhance Spin-Crossover Hysteresis in a Fe(II) Hofmann-Type MOF

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Controlling bistability in Fe(II) spin-crossover (SCO) metal–organic frameworks (MOFs) remains a key challenge for their implementation in functional devices, as the width of thermal hysteresis is often limited by weak cooperative interactions[1]. Here, we demonstrate that guest-induced chemical pressure is an effective and reversible strategy to enhance bistability in the Hofmann-type framework $[Fe(pz)Pd(CN)_4]$. Owing to their porosity and flexibility, MOFs enable host–guest interactions that mimic external stimuli such as pressure[2]. Vapor-phase iodine uptake induces lattice compression while preserving the framework integrity, strengthening elastic interactions between Fe(II) centers. As a result, partial iodine loading produces multistep and asymmetric SCO behaviour, whereas full saturation leads to a record-wide and symmetric thermal hysteresis of up to 120 K, exceeding typical values reported for related systems[3]. The process is fully reversible, ensuring reproducible switching. These results highlight guest incorporation as a powerful, non-destructive approach to tune SCO properties and design multifunctional materials for sensing and memory applications. Furthermore, this strategy provides a general route to control cooperative phenomena in porous coordination frameworks without altering their chemical composition, opening new opportunities for the rational design of responsive and adaptive molecular materials.

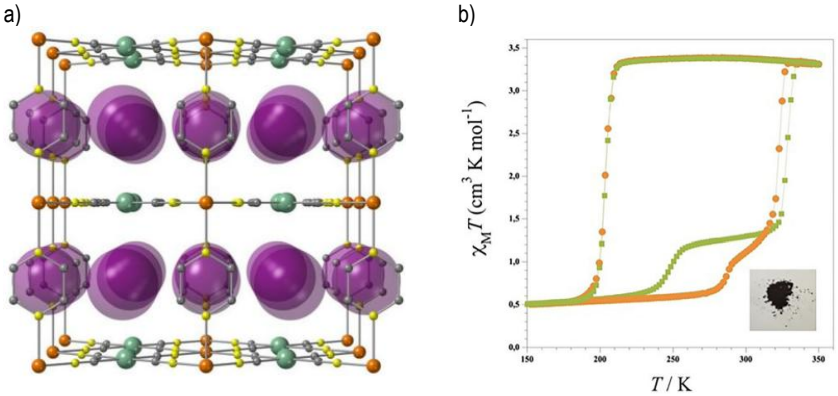

Figure. a) Illustration of the structure of $[Fe(pz)Pd(CN)4]@I_2$. b) Temperature-dependent magnetic susceptibility (χMT vs. T) of $[Fe(pz)Pd(CN)4]\cdot 0.5\ I_2$, where green curve corresponds to the first cooling–heating cycle, while the orange curve corresponds to the second thermal cycle.

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Designing of small molecules for the degradation of 3D DNA structures

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Beyond the classical double helix, non-canonical structures like G-quadruplexes (G4) play critical roles in various scientific domains. G4s form through the stacking of G-quartets—planar arrangements of guanines held by Hoogsteen hydrogen bonds and stabilized by sodium and potassium cations, in guanine rich DNA and RNA sequences.[1] In the last decades, putative G4-forming sequences have been identified in key genomic regions linked to cancer and neurodegeneration and moreover, these structures have emerged as epigenetic controllers. In the field of neurodegeneration, amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD) have been characterized by the presence of tandem of the hexanucleotide repeats GGGGCC in the *C9orf72* gene, which folds into the alternative G-quadruplex. Several studies have highlighted the relationship between the aberrant formation of these alternative structures and the severity of the diseases. Therefore, novel approaches have been proposed to ameliorate the neurodegeneration, including the degradation of these G4s arise in the *C9orf72* gene.

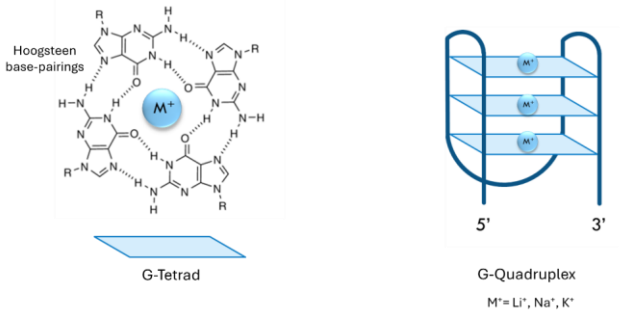

Figure 1. G-quadruplex structure.

In this work, we have prepared a portfolio of bimodal molecules, containing two modules: (i) a well-known G4 binder and (ii) a RNA cleaver. We have prepared two families of G4 binders, polyamine derivatives and nickel-salophen complexes, each of them functionalized with imidazole groups, which works as RNA cleaver.[2] The portfolio of ligands includes alkyl spacer chains of varying lengths, ranging from four to six carbon atoms. Our aim is to evaluate them in cell culture to investigate their capacity for G4 degradation. Lastly, a secondary objective of to determine the optimal the chain length for efficient degrade alternative G4s, establishing a structure-activity relationship between chain size and degradation potency.

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Mechanosensitivity in dithia-helicenes through thermopower and conductance

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Helicenes are chiral carbon-based molecules of interest in diverse fields, including electron transport in molecular junctions. Recently, our research into dithiahelicene molecular junctions revealed that electronic conduction is governed by off-resonant transport mechanisms [1]. In this regime, conductance decays exponentially with the energy offset between the molecular HOMO/LUMO levels and the metal work function; specifically, the HOMO level of dithiahelicenes is aligned within 1 eV of the gold work function.

Further research on related helicenes has shown that their electronic properties can be mechanically tuned [2]. Break-junction experiments allow for the application of force to either compress or stretch a single helicene, providing a method to modulate the conductance and thermopower of the junction. Motivated by this, the group of Prof. Nicolas Agraït measured the thermopower in endo/exo-dithia[10]helicenes and endo/exo-dithia[11]helicenes. We performed DFT transport calculations using the Non-Equilibrium Green's Functions (NEGF) method to characterize thermopower variations under mechanical deformation. These metrics allow us to characterize the alignment of the gold work function relative to the HOMO level across different elastic conformations.

Although the conductance is nearly identical across these dithiahelicene species [1], our characterization of the thermopower reveals distinct differences between isomers in both compressed and stretched states. Specifically, exo isomers exhibit a sign reversal in the Seebeck coefficient—transitioning from positive to negative—while endo isomers maintain a positive coefficient throughout the process. This suggests either a fundamental difference in HOMO-LUMO alignment or a highly consistent variation in mechanical conformation between these species. We explore these possibilities in this presentation.

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Multifunctional cascade enzyme nanoplatform for enhanced tumor starvation under hypoxic conditions

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Metal-organic frameworks (MOFs) are a class of hybrid porous materials composed of metal ions or clusters linked by organic ligands. Lately, they have gained attention as they are promising candidates for biomedicine applications. However, its clinical translation is limited due to poor colloidal stability, potential systemic toxicity and rapid immune clearance. In this regard, extracellular vesicles (EV) show an inherent ability to traverse biological barriers, higher stability and low immunogenicity, making them as well ideal candidates for enhancing the biocompatibility and targeting precision of nanomaterials [1]. The harsh synthetic conditions typically required for MOF assembly avoid the *in situ* encapsulation of sensitive biomolecules. Recent advances in our group have demonstrated the capability to carry out the one-pot protein encapsulation, developing a synthetic method of MOFs under physiological conditions. In this study, we propose the use of EV coating UiO-66 as protein nanocarriers to improve starvation treatment in hypoxic tumors as we can report its biocompatible synthesis, ensuring suitability for labile biomolecular cargo [2].

One of the main hallmarks of cancer status is Warburg effect, which states that, compared to their normal counterparts, cancer cells are more susceptible to glucose shortages. Although starvation therapy triggered by glucose oxidase can be a promising route, the lack of oxygen into hypoxia prevalent solid tumors often circumvents nutrient-deprivation efforts. Thus, the most direct solution is to increase the therapeutic effect by supplementing oxygen to relieve hypoxia.

Furthermore, the therapeutic use of free glucose oxidase (GOx) is limited by its short lifetime in the body, and although efforts employing nanocarriers have improved these features, off-target toxicity is a relevant barrier as it induces unregulated starvation and acidifies the microenvironment via gluconic acid accumulation [3]. We hypothesize that the co-encapsulation of GOx and catalase (CAT) within the UiO-66 creates a self-sustaining catalytic loop that triggers a synergistic anticancer effect, relying on oxygen recycling and targeting the described metabolic adaptation. Besides, UiO-66 coating with own A549 EV could encourage homotypic recognition, thus treatment of the same cell type from which the vesicles were extracted and avoid unspecific cell death promote by pH decreased via extracellular gluonic acid formation.

EVs-coated UiO-66 nanocarriers have demonstrated the highest stability in relevant physiological media. These studies performed via HPLC and DLS demonstrated stronger protection of EVs versus reported coating molecules, such as PEG. Additionally, endosomal escape by EV-MOF has been analyzed in a confocal microscope and protective extracellular glucose consumption was demonstrated by TMB-peroxidase activity assay. Lastly, biosafety of the nanocarrier as well as effectiveness under normoxic and hypoxic conditions will be soon evaluated.

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Ti-based MOFs as Biomimetic Artificial Metalloproteases

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Metal–organic frameworks (MOFs) offer a programmable platform that embeds catalytic metal–oxo nodes within a tunable porous architecture, enabling the capture of substrates and enzyme-like catalysis under aqueous conditions [1]. While Zr-based MOFs have established key design principles for artificial proteases, proteolytic catalysis in titanium-based frameworks remains largely unexplored. Here, we investigate the heterometallic titanium MOFs MUV-101(Fe) and MUV-101(Zn) as biomimetic and recyclable artificial metalloproteases for controlled protein hydrolysis.

Our aim is to establish structure–function relationships governing activity, selectivity, and robustness in these systems using ovalbumin as a model protein substrate. We hypothesize that the distinct Ti–Fe and Ti–Zn node compositions encode different cooperative effects analogous to those of dinuclear enzymatic sites, including water activation, amide carbonyl polarization, and transition-state stabilization [2], which should translate into measurable differences in proteolytic behavior.

To test this, we compare MUV-101(Fe) and MUV-101(Zn) through catalytic and structural analyses, focusing on ovalbumin adsorption, hydrolysis, and fragment recovery. These analyses utilize UV–visible absorbance spectroscopy, circular dichroism, SDS–PAGE electrophoresis, and PXRD. In parallel, we evaluate an integrated capture–process–recover workflow relevant to proteomics, assessing the ability of these materials not only to promote protein cleavage but also to control substrate binding and product release.

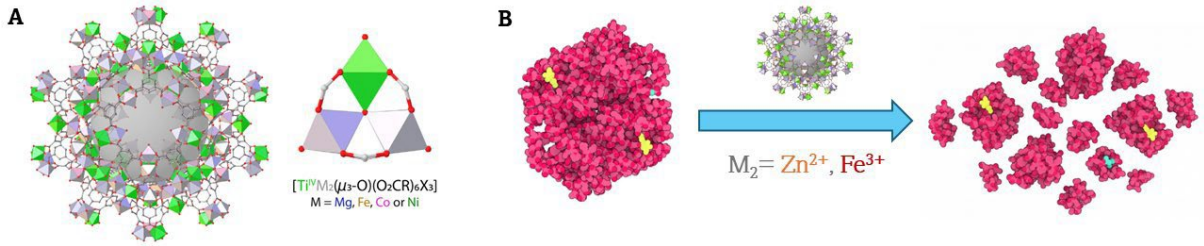

Figure 1. MUV-101 Heterometallic Titanium Organic Frameworks and Protein Hydrolysis. (A) Structure of the family of mesoporous materials MUV-101 (left) from the interlinking of heterometallic titanium clusters (right) and trimesate linkers. (B) Schematic illustration of the proteolytic hydrolysis of ovalbumin mediated by Fe- and Zn-based MUV-101 materials, resulting in fragmentation of its native structure.

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Close-Space Sublimation for Perovskite/Silicon Tandem Solar Cells

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Perovskite/silicon tandem solar cells are a promising route to overcome the efficiency limits of single-junction silicon devices. For their large-scale implementation, scalable fabrication methods for the perovskite top cell are needed. In this context, close space sublimation (CSS) is an attractive vapour-phase approach because it enables solvent-free processing and is compatible with scalable manufacturing [1]. Recent works have shown promising results for CSS in single-junction perovskite solar cells [2,3], while its application in perovskite/silicon tandems is still limited. In this work, CSS is used to fabricate the perovskite layer in tandem solar cells with a silicon bottom cell. The process is based on the conversion of an evaporated inorganic precursor by exposure to organic vapours under controlled source and substrate temperatures, chamber pressure, and source-to-substrate spacing. The fabrication procedure, the main parameters affecting precursor conversion and film formation, and first results from initial batches in tandem-compatible device structures are discussed.

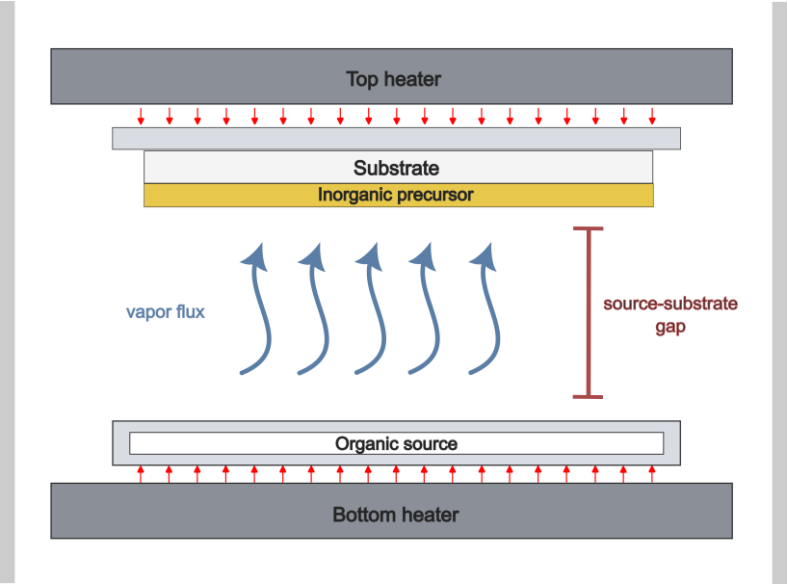

Figure 1. Schematic of the close space sublimation process for perovskite conversion.

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Synthesis of acylhydrazone MOFs

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Metal-organic frameworks (MOFs) are a new type of inorganic-organic hybrid crystalline materials formed by the ordered assembly of metal ions or clusters connected by organic ligands with a high potential thanks to their tailorable topologies, adjustable pore sizes, and exceptionally high specific surface areas.[1] The incorporation of uncoordinated acylhydrazone groups into a MOF provides highly versatile interaction sites that enable several functional applications like selective gas adsorption [2] or Highly Sensitive Chemical Sensing [3]

This work presents the synthesis and characterization of a series of MOFs based on heterotopic ligands and different metal centers (mainly zinc). The obtained materials were characterized using various techniques like powder X-ray diffraction (PXRD) single crystal XRD (SC-XRD), infrared spectroscopy (IR) or thermogravimetric analysis (TGA).

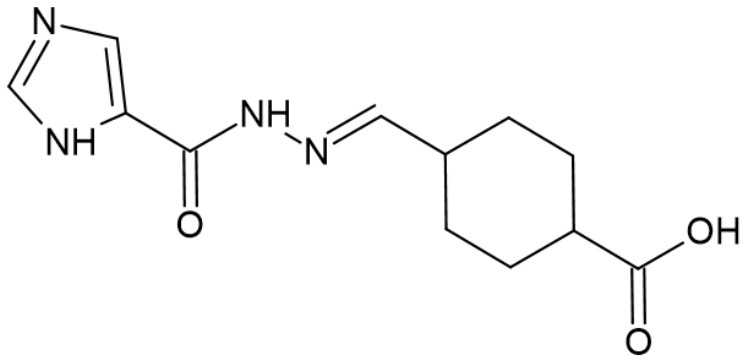

Fig 1: Example of acylhydrazone ligand

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Pressure-Activated Spin crossover in Flexible metallomesogens

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Spin crossover (SCO) is a process where materials exhibit reversible switching between high-spin (HS) and low-spin (LS) states in response to external stimuli such as temperature, light or pressure, offering unique opportunities for sensing, memory devices, actuators and molecular electronics.[1] This process is well understood in crystalline solids, but extend this capability to soft and dynamically structured materials is very difficult, because molecular flexibility and structural disorder suppress the intermolecular cooperativity required for the spin-state switching, leading to suppress or inhibited transitions.[2] We report a family of Fe(II) metallomesogens where thermally induced spin crossover is suppressed across crystalline and liquid-crystalline phases proved by magnetometry measurements, and exhibit a fully reversible pressure-induced spin transition at different pressures in the GPa scale demonstrated by variable-pressure Raman spectroscopy. Also, by differential scanning calorimetry (DSC) the structural transitions are observed and identificated using a polarised optical microscope (POM). These results define a mechanically gated spin crossover mechanism, in which molecular flexibility suppresses the spin-transition under thermal stimuli while enabling it under mechanical compression with the restauration of the intermolecular coupling.

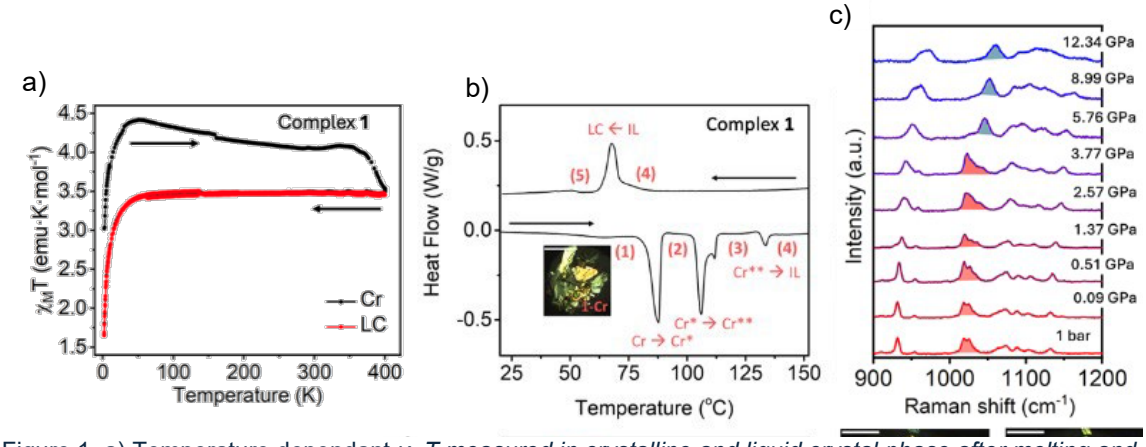

Figure 1. a) Temperature dependant $\chi_M T$ *measured in crystalline and liquid crystal phase after melting and cooling down room temperature, b) Differential scanning calorimetry measurements highlighting the phase transitions and corresponding states, c*) variable pressure Raman spectra for alkyl chain complex.

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Modulating WSe2 photoluminescence through ferroelectric polarization coupling in a van der Waals heterostructure

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The atomic thickness of 2D materials provides an ideal platform for novel quantum phenomena to manifest within van der Waals heterostructures. Furthermore, the integration of 2D ferroelectric materials with 2D photoelectric materials via interface engineering enables fundamental investigations into controlled doping and device integration in layered semiconductors. In this study, we design a novel device architecture to investigate the voltage-controlled ferroelectric polarization of $CuInP_2S_6$ (CIPS) through interface coupling with a WSe_2 semiconductor. Our setup allows for the application of electric fields in both in-plane and out-of-plane directions while simultaneously measuring photoluminescence (PL) spectra. Through this design, we expect to observe in situ modulations of the WSe_2 PL spectra under varying CIPS polarization states. Ultimately, this work seeks to enhance the fundamental understanding of ferroelectric-semiconductor coupling, paving the way for future applications in compact, non-volatile memory devices.

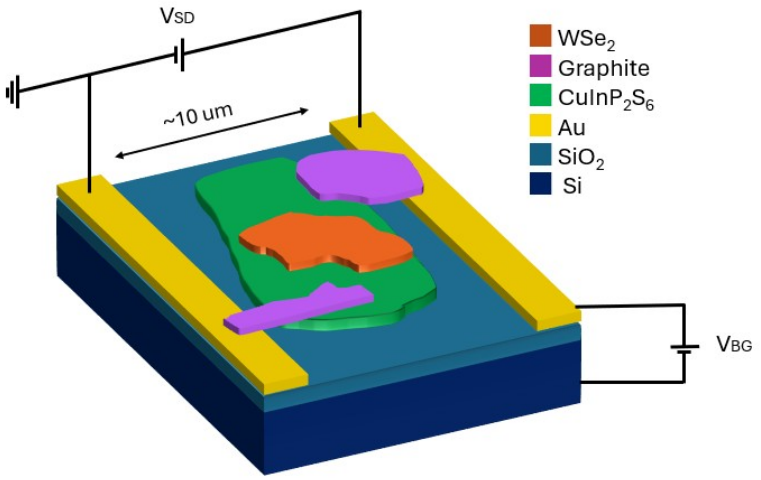

Figure I: $CuInP_2S_6/WSe_2$ heterostructure

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Tailoring 1D Anilato-Based Coordination Polymers: Synthesis, Structural Studies, and Selective Sensing of Volatile Organic Compounds (VOCs)

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This work reports the synthesis and characterisation of two new copper(II) coordination compounds with the formula $[Cu(C_6O_4X_2)(H_2O)_2]\cdot 2DMF$ (X = Cl, Br). These materials, obtained by the layering technique, are isostructural 1D linear coordination polymers (Figure 1). The study of their reactivity against a diverse range of Volatile Organic Compounds (VOCs), including acids, bases, and neutral solvents, is in progress. Preliminary results, confirmed by X-ray powder diffraction, demonstrate a selective response, highlighting the promising potential of these compounds for future applications as chemical sensors.

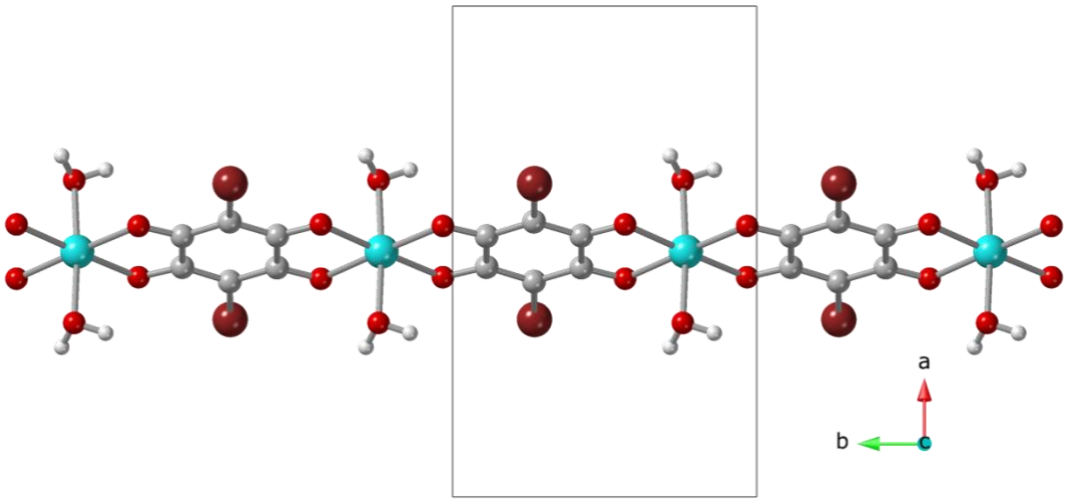

Figure 1. View of the chain structure of compound $[Cu(C_6O_4Br_2)(H_2O)_2]\cdot 2DMF$

Strongly bound excitons in the layered material BiI_3: a thickness and temperature dependent study

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Excitons in two-dimensional (2D) layered materials exhibit extraordinary stability, often persisting at room temperature due to strong quantum confinement and reduced dielectric screening. This robustness drives emerging technological advancements in optoelectronics, quantum optics, and the rapidly growing field of valleytronics [1]. Excitons in bismuth triiodide (BiI_3) feature unusually strong binding energies, predicted to approach 900 meV in the monolayer limit [2] due to its heavy element composition, making this material an ideal platform for exploring excitonic phenomena, featuring a giant spin-orbit coupling. Furthermore, BiI_3 visible-range bandgap (~2 eV) and flat bands near the Fermi level facilitate the formation of a rich landscape of excitonic states [3] for example surface excitons, or long-lived dark excitons characterized by a null electric dipole.

In this work, we investigate the layer-dependent optical properties of BiI_3 using transmittance and photoluminescence (PL) spectroscopy, demonstrating that its strong excitonic character is preserved at room temperature. Further extending our measurements to cryogenic temperatures, we resolve the fine structure of the emission spectra, successfully distinguishing intrinsic free-exciton transitions from localized defect-bound states. Finally, we analyze the temperature-dependent evolution of these PL features across different layer thicknesses to extract more insights into the exciton-phonon coupling mechanisms governing this material.

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Systematic Raman spectroscopy study of Ni layered hydroxide: Influences of disorder

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As climate change induced meteorological disasters become more prominent worldwide, the cry for decarbonisation of industry, transport and the energy sector grows louder. A high-profile pathway towards this goal is the deployment of renewable energy and the subsequent conversion to energy carriers. A critical factor in these conversions is the availability of suitable materials, among which Layered Hydroxides (LH) show great promise in both hydrogen production and battery applications. Additionally, the LHs have gained interest in mitigating other human induced environmental problems such as soil remediation and water purification.[3] Therefore, a thorough understanding of these materials is essential for further development towards societal incorporation.

LHs come in three phases, the α-phase (Simonkolleite-like), β-phase (brucite-like) and layered double hydroxides (LDH)[4], where the LDH is the most promising due to their chemical versatility. However, current reports show discrepancies in the interpretation of characterisation techniques like Raman spectroscopy largely due to the absence of systematic research in the literature. The versatile LDH phase is a non-ideal starting point in understanding the dynamics of such structures, hence the β-phase is studied. In this straightforward LH phase, subtle deviation in spectral features such as peak shifts and relative intensities are not yet correlated with crystallographic or material properties.

In this study, Raman spectroscopy is performed systematically on high crystalline as well as disordered beta-Ni LH samples. In addition, the same structure with different cations are synthesized and studied to understand the lattice dynamics. Through this dual approach, we aim to develop a comprehensive understanding of how both cation type and structural disorder influence the material. This will provide a strong foundation for interpreting the more complex and application-oriented LDH structures.

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Conductivity and Magnetization Switching in Ni-Fe Cyanido-Bridged Coordination Polymer Through H_3O^+/NH_4^+ Exchange

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Currently, considerable attention is given to molecule-based proton conductors, such as metal-organic frameworks (MOFs) or coordination polymers (CPs), which present a wide range of functionalities. In particular, cyanido-bridged CPs are promising candidates for solid-state conductors, exhibiting high proton conductivities reaching up to 10^{-3} S cm^{-1} [1] and combining them with other switchable functionalities such as photomagnetism [2,3]. Herein, we focus on a family of CPs: A[Ni(cyclam)]-[Fe(CN$_6$)]·5H$_2$O (A = NH_4^+ /**1NH$_4^+$**/, H_3O^+ /**2H$_3$O$^+$**/). Compound **1NH$_4^+$** exists in two valence states containing exclusively Ni^{II}-Fe^{III} (HT) or Ni^{III}-Fe^{II} (LT) sites, as a consequence of electron-transfer phase transition (ETPT) [4], which is controlled by temperature, pressure, or light; however, it is switched off by dehydration. In this study, we discovered that an ion-exchange - NH_4^+ for H_3O^+ - achieved by leaching the crystals of **1NH^{4+}** in an acidic solution also switches off the ETPT. Conversely, sorption of NH_3 onto the resulting **2H$_3$O$^+$** recreates the ammonium cations (**3NH$_4^+$**) and restores ETPT. The ETPT induces a simultaneous switching of proton conductivity and activation energy, with σ changing from 3.6×10^{-7} (LT) to 1.0×10^{-8} S cm^{-1} (HT) and a corresponding change in E_a from 0.54 to 0.26 eV (295 K, 50% RH). In contrast, **2H$_3$O$^+$** shows no conductivity switching due to the absence of ETPT, which is reestablished in **3NH$_4^+$** upon NH_3 sorption. Therefore, **1NH$_4^+$** acts as a multifunctional molecular switch exhibiting room-temperature bistability of magnetic and H^+-conducting properties. To the best of our knowledge, this is the first CN-bridged system exhibiting changes in proton conductivity via ETPT.

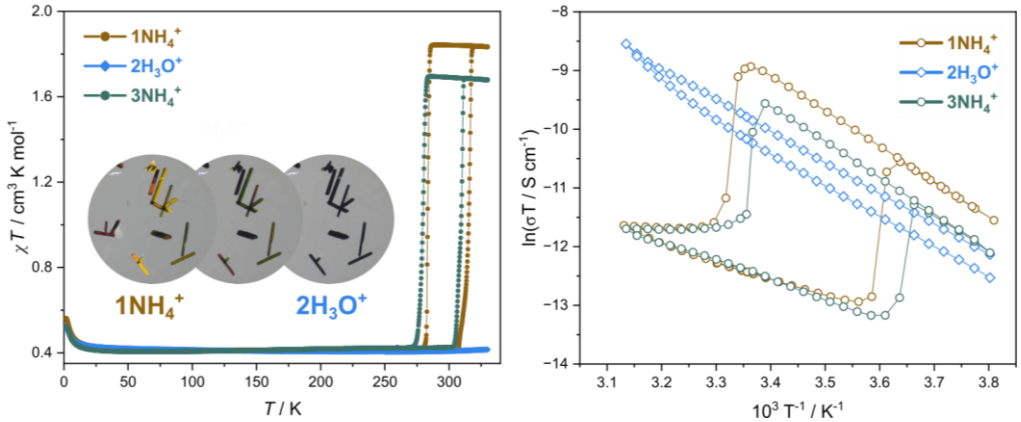

Figure 1. Temperature dependence of the product of magnetic susceptibility and temperature (χT, left), and ln(σT) vs T^{-1} plots (right) for **1NH$_4^+$**, **2H$_3$O$^+$**, and **3NH$_4^+$**.

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Quantum Transport Measurements in Single-Molecule Glycerol Junctions: A Machine Learning Analysis

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Over the past two decades, break-junction (BJ) experiments have become a standard method for studying molecular electronics [1]. Traditionally, these experiments are conducted either in cryogenic vacuum [2] or at room conditions [3]. Both methods have significant drawbacks: cryogenic setups are costly, time-consuming, and technically demanding, whereas room-temperature measurements often suffer from contamination and environmental noise. To overcome these issues, we utilize a liquid environment not only as a dispersion medium for target molecules, but also as a protective shield to facilitate room-temperature BJ experiments with minimized contamination. Using semi-supervised clustering machine learning algorithms, we characterized glycerol molecular junctions formed between gold electrodes under a glycerol meniscus. By isolating the background conductance response of the glycerol, we successfully established a methodology that allows for the precise study of other target molecules in solution.

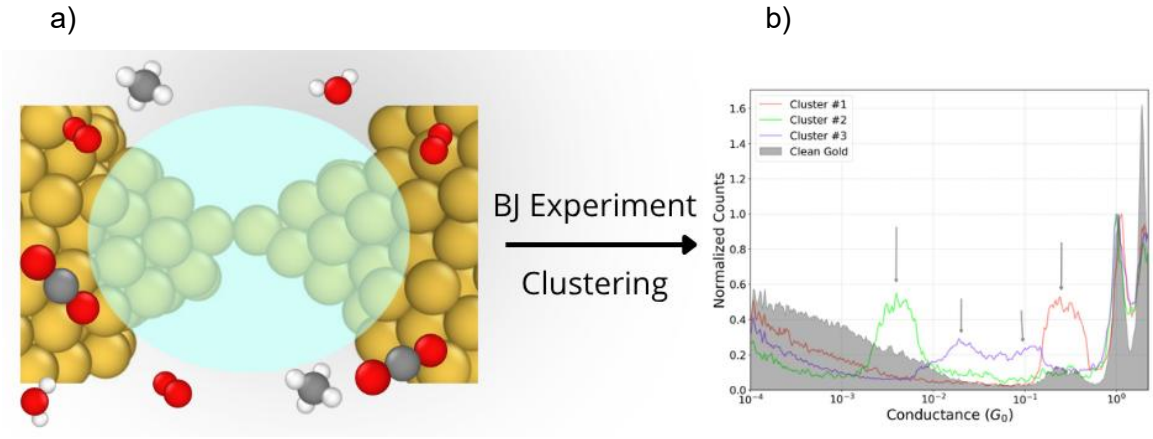

Figure 1. (a) Schematic representation of the nanojunction shielded from external contamination by glycerol. (b) Clustered results of a BJ experiment for glycerol measured between gold electrodes.

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Sequential Vacuum Deposition of Cs/Cl-Alloyed $FAPbI_3$ Perovskite Absorbers

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Sequential vacuum deposition represents a highly scalable solvent-free pathway for the industrial manufacturing of perovskite solar cells, allowing for precise thickness control and decoupled crystallization [1]. Through this technique, formamidinium lead iodide ($FAPbI_3$) has emerged as a premier absorber candidate due to its optimal bandgap and exceptional thermal stability. However, obtaining phase-pure photoactive α-$FAPbI_3$ via this route remains challenging. The inherent thermodynamic instability of the material and the high density of the co-evaporated inorganic layer often restrict the complete solid-state reaction, ultimately leading to the formation of the photoinactive yellow δ-phase [2].

In this work, we investigate the phase transition of sequentially deposited perovskite films employing a co-evaporated inorganic layer of PbI_2 alloyed with CsI and $PbCl_2$, followed by the thermal evaporation of formamidinium iodide (FAI). The incorporation of Cs^+ and Cl^- is well-documented to relax crystal strain, lower the formation energy of the α-phase, and act as transient stabilizers during the structural conversion [3]. Building upon these principles, this study focuses on facilitating a highly efficient solid-state reaction between the dense inorganic template and the organic vapor. By systematically optimizing the deposition parameters and the subsequent conversion process, we aim to promote a complete microstructural evolution toward the desired 3D perovskite structure. Through comprehensive structural and optical characterization, we identify the critical factors required to suppress the δ-phase and other intermediate subproducts. Ultimately, this work provides practical insights into achieving highly reproducible, phase-pure α-$FAPbI_3$ absorbers, contributing to the reliable manufacturing of vacuum-processed solar cells.

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Competing spin correlations and their spectra between magnetic molecules coupled to superconducting leads

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The study of magnetic impurities in superconductors is a fundamental challenge in condensed matter physics, crucial for understanding phenomena like in-gap states such as Yu-Shiba-Rusinov (YSR) states. Systems with multiple impurities can potentially host exotic ground states relevant for topological quantum applications. Accurate numerical methods like the numerical renormalization group are computationally demanding for solving more than two impurity levels. Recently, an efficient impurity solver was proposed, based on the exact diagonalization of a single impurity connected to discretized superconducting reservoirs [1]. In this work, we extend this model to the case of two magnetic impurities coupled to BCS superconductors. By exact diagonalization of the resulting tight-binding Hamiltonian, we study the competition between the impurity-superconductor coupling and the impurity-impurity exchange to form a singlet with the bath or a singlet between the impurities themselves. The results reveal the evolution of YSR states and spin correlations, showing transitions between distinct quantum phases driven by this competition.

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Dry-Processed Wide-Bandgap Perovskite Solar Cells

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Metal halide perovskites have emerged as highly tunable optoelectronic materials for next-generation photovoltaics. Wide-bandgap perovskites (~1.8 eV) are essential for efficient all-perovskite tandem solar cells, as they enable higher open-circuit voltages (V_{oc}), but at the expense of reduced short-circuit current density (J_{sc}) [1]. In practice, these materials also suffer from a pronounced V_{oc} deficit caused by defect formation, photo-induced halide segregation, and energy level misalignments. Here, we investigate the fabrication of wide-bandgap perovskites via thermal co-evaporation, a scalable solvent-free technique that offers precise control over complex stoichiometries. Bandgap tuning in a triple-cation system (CsFAMAPbIBr) is achieved by systematically adjusting the bromide-to-iodide ratio during deposition. To mitigate the V_{oc} deficit, we introduce chloride through a methylammonium chloride (MACl) pellet source [2]. This approach enables improved film quality and reduces non-radiative recombination, leading to enhanced device performance. Our results highlight a viable pathway toward robust, high-efficiency all-perovskite tandem solar cells. single spaced paragraph.

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Photochemical and Photophysical Properties of Carbon Nano-Onions Towards Combined Phototherapy Applications

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Carbon nano-onions (CNOs) are concentric, graphitic carbon nanostructures that stand out for their high surface-to-volume ratio, stability, and excellent biocompatibility. These features have positioned them as promising candidates in biomedical research, particularly in areas like drug delivery, imaging, and cancer treatment.

In our work, we focus on exploring the potential of CNOs in photothermal (PTT) and photodynamic (PDT) therapies. When exposed to near-infrared light, CNOs exhibit efficient heat generation and can produce reactive oxygen species (ROS), opening the door to combined therapeutic approaches. The photothermal conversion efficiency observed was notably high, even when compared to other well-known carbon nanomaterials. At the same time, we confirmed their ability to generate ROS under irradiation, which adds an oxidative stress mechanism that can be harnessed in cancer therapy.

Building on these encouraging results, we are also working toward enhancing the targeting capabilities of these nanomaterials. To achieve this, we are developing strategies to graft DNA-based structures, such as aptamers, onto the surface of the CNOs. These oligonucleotides can recognize and bind specific biomarkers on cell membranes, potentially allowing for more selective accumulation of CNOs in diseased tissue while minimizing side effects on healthy cells.

Together, these efforts aim to establish CNOs as passive drug carriers and active, multifunctional platforms for next-generation cancer therapies. By combining efficient light-responsive behavior with molecular targeting, we envision CNOs as key components in future theragnostic systems—capable of diagnosing, treating, and monitoring disease in a single step.

Towards Anthraquinone-Phosphonate Metal-Organic Frameworks

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Phosphonate-based metal-organic frameworks (MOFs) are of great interest for enhancing the proton or ionic conductivity of these materials and for the design of mixed ionic-electronic conductors.[1] Furthermore, the use of redox-active ligands such as anthraquinone shows significant promise for energy storage applications due to their high theoretical specific capacity and excellent electrochemical reversibility.[2]

This work presents the synthesis and characterization of a series of MOFs based on redox-active anthraquinone-phosphonate ligands and lanthanum metal centers. The obtained materials are characterized using various techniques, including powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), and cyclic voltammetry (CV). Additionally, this study evaluates how different reaction parameters (temperature, time, synthesis method, and reagent concentration) influence the morphology, degree of crystallinity, and phase formation of the resulting MOFs.

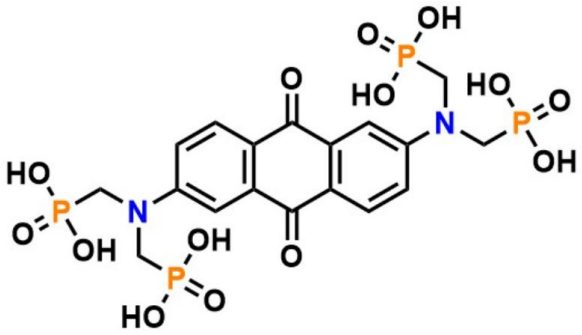

Fig 1: Anthraquinone-phosphonate ligand used for the synthesis of MOFs.

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UIO-66 as platform for in situ encapsulation of nucleic acids and gene delivery

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Metal-organic frameworks (MOFs) are porous crystalline materials formed through the coordination of organic ligands with metal centers, such as ions or clusters, creating extended structures [1].These materials exhibit distinctive features such as chemical tunability, high porosity and physico-chemical stability. In addition, their high cargo loading and biodegradability in physiological media, render them particularly suitable as platforms for the encapsulation of biomolecules, thereby contributing to their growing relevance in biotechnological applications [2-3].

Leveraging these inherent characteristics, a biocompatible synthesis of the extensively studied UIO-66 has been developed in our research group, using 1,4-benzene dicarboxylic acid (BDC) as the organic ligand and a preformed Zr(IV) cluster as the metal source. The mild and biocompatible reaction conditions enable the in situ encapsulation of biomolecules, allowing their incorporation into the framework [4].

In the present study, the biocompatible synthesis of UIO-66 will be employed for the in situ encapsulation of nucleic acids. In order to optimize the encapsulation process, a scale-down approach will be implemented, focusing on maximizing both encapsulation efficiency and cargo loading for these high-value biomolecules. Furthermore, various surface coatings will be investigated to enhance the stability of the MOF under physiological conditions and to promote cellular uptake. These strategies are expected to highlight the potential of UIO-66 as a versatile platform for the encapsulation and delivery of nucleic acids in biomedical applications.

Figure 1. Schematic representation of the in situ encapsulation of nucleic acids with UIO-66.

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Theoretical description of samarium(III) complexes: versatile simulation of optical and magnetic properties

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Intensive development of advanced luminescent and magnetic materials based on metal complexes has created an increasing demand for robust theoretical approaches capable of supporting and rationalizing experimental findings [1,2]. In particular, there is a need for computational methods that offer a balance between accuracy, reliability, and practical accessibility, while effectively capturing complex phenomena such as chiroptical activity, luminescence, and magnetic behaviour. In this contribution, we present a comprehensive theoretical investigation of Sm(III) complexes bearing chiral *S*- or *R*-2,2′-bis(diphenylphosphino)-1,1′-binaphthyl (*S*-/*R*-$BINAPO_2$) ligands, with the coordination sphere completed by $[Ag^{I}(CN)_2]^-$ metalloligands. The computational study employs a Complete Active Space Self-Consistent Field (CASSCF) method augmented with Second-Order Perturbation Theory (CASPT2) to achieve an accurate description of electronic structure [3]. The applied methodology enables the simulation of a wide range of optical and magnetic properties, including circularly polarized luminescence (CPL) spectra (Figure 1). The results demonstrate the capability of advanced multi-reference approaches to reliably describe the interplay between the electronic structure and spectroscopic properties in lanthanide(III)-based molecular systems, highlighting their potential as predictive tools in the design of functional molecular materials.

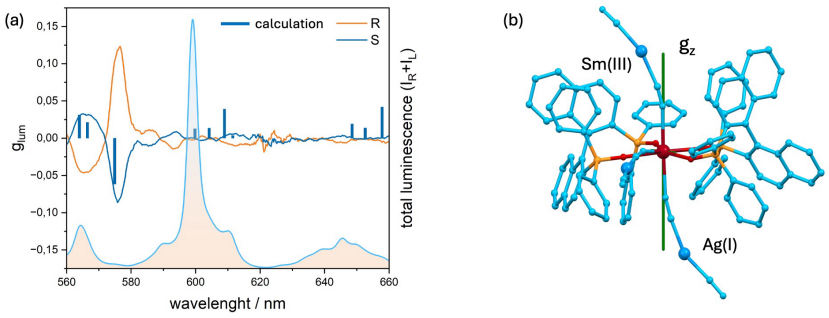

Figure 1. The experimental photoluminescence (total luminescence) and circularly polarized luminescence (CPL, in the form of g_{lum}) spectra with corresponding calculated CPL intensities (a), and the visualization of the crystal structure of the investigated Sm(III)-Ag(I) coordination polymer incorporating the studied $\{Sm^{III}(BINAPO_2)_2[Ag^{I}(CN)_2]\}^-$ complexes, shown with a principal axis of magnetization for Sm(III) ions (b).

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Defect Engineering in Multivariate Metal–Organic Frameworks toward versatile applications

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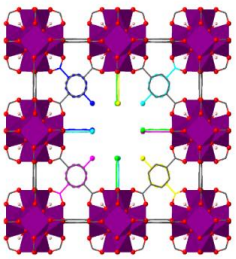
Multivariate Metal–Organic Frameworks (MTV MOFs)[1] [2] represent an advanced class of porous crystalline materials in which multiple organic linkers and/or metal nodes are integrated within a single framework. This multicomponent design enables the creation of chemically heterogeneous pore environments, giving rise to cooperative and emergent properties that surpass those of single-component analogues.

Building on this concept, multivariate modulation [3] [4] introduces an additional level of structural control by incorporating functional modulators during synthesis. Beyond simply generating compositional diversity, this strategy enables deliberate defect engineering, allowing precise regulation of missing-linker or missing-cluster defects while simultaneously tailoring the chemical microenvironment of the pores. In conventional MTV MOFs, the incorporation of multiple linkers can reduce accessible porosity due to steric hindrance or partial pore blockage. In contrast, modulation-driven defect engineering can restore and even enhance pore accessibility by creating additional free volume and exposed active sites.

The combination of multivariate design and controlled defect formation creates synergistic adsorption sites and promotes complementary interactions with target molecules. As a result, modulated defective MTV MOFs emerge as highly promising materials for environmental remediation, particularly in water purification and air treatment, where selective adsorption, high uptake capacity, and robustness under operating conditions are essential [5] [6].



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Tuning Spin-Crossover Behaviour for Pressure-Induced Thermal Effects

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Barocaloric cooling, based on pressure-induced temperature changes, is a promising solid-state alternative to conventional refrigeration technologies. Materials exhibiting large entropy changes, low hysteresis, and significant volume variation during phase transitions are key to achieving efficient barocaloric effects. Spin-crossover (SCO) compounds are particularly attractive in this context due to their switchable electronic states and structural flexibility.[1]

In this work, we present the synthesis, structure, and characterization of a family of iron(II) SCO complexes, and demonstrate how ligand field design enables precise tuning of their spin transition behaviour. By modifying the ligand environment, we control both the transition temperature and its response to applied pressure. Magnetic measurements under variable temperature and pressure reveal a significant modulation of the spin transition, highlighting the potential of these materials for low-pressure, near room-temperature barocaloric applications. These results provide useful guidelines for the rational design of molecular barocaloric materials.

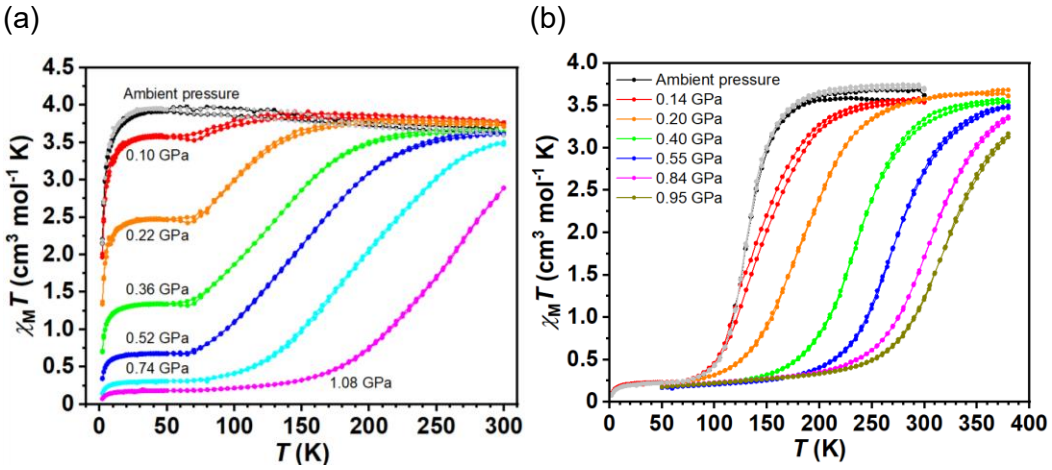

Figure 1. Variable-temperature magnetic curves at different applied pressures for Fe complexes, where the anion is SCN (a) and SeCN (b).

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Polymer electrolyte membranes

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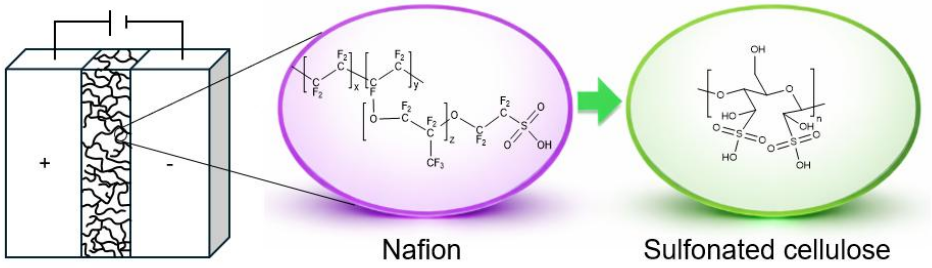
Figura 1. Traditional Nafion-based membranes VS. sulfonated cellulose membranes.



Ion selective membranes constitute a key component in several technologies for scale energy storage, such as redox flow batteries. Currently, these membranes are made of synthetic polymers and dominated by Nafion, the perfluorinated sulfonic material, which is particularly problematic from a sustainability perspective and its high cost. There is strong interest in replacing these traditional ion exchange membranes by non-fluorinated bio-based and renewable materials. Cellulosic nanomaterials can be suitable due to their abundancy, low cost, processability and the versatility of functionalization methods available, which can enhance their ionic conductivity.[1]

In this work, we present a simple and sustainable approach based on the periodate oxidation of cellulose followed by a sulfonation reaction,[2] aimed at preparing membranes of micrometric thickness via solution casting. A series of samples was obtained by varying the degree of sulfonation and the amount of polyethylene oxide, a polymer known to foster mechanical properties and ionic conductivity by providing a flexible medium that solvates and mobilizes cations for efficient transport.[3]

The composition and thermal stability, chemical modification, and surface morphology of the membranes were characterized by elemental analysis and TGA, ATR-IR and SEM, respectively. The water uptake was determined gravimetrically after a fully immersion of the membranes in zinc-based electrolyte. Further characterization of the membranes, along with detailed conductivity studies, is planned for future work.

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Multifunctional molecular materials based on lanthanide complexes with dithiocarbamate ligands

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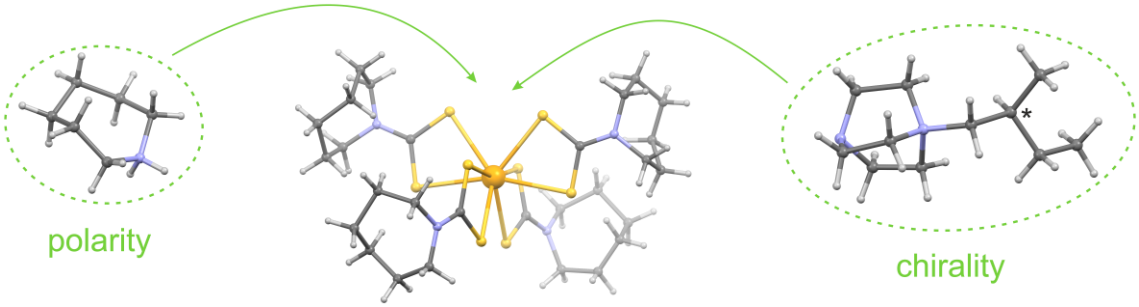
Molecular materials attract a lot of scientific attention considering their easy tunability with the molecular building blocks synthetic approach. With rationally selected organic ligands of almost infinite variety and metal ions with well-defined intrinsic properties, novel molecular solids bearing designable photoluminescent, optical (including chirality-related and non-linear ones), magnetic, and electrical functionalities can be obtained [1]. Such strategy allows the synthesis of multifunctional materials that are considered for applications in sensors, bioimaging, electronics, and molecular switches [2,3]. In this context, lanthanide(III) complexes are well-known for their photo-luminescent and magnetic properties [4,5]. Following this line, here, we report the exploration of lanthanide complexes with dithiocarbamate ligands as the molecular building blocks for multifunctional hybrid ionic salts. The obtained materials can be described with the general formula of $(X)[Sm^{III}(L)_4]$ (X = an organic polar or a chiral cation, L = a dithiocarbamate-type ligand, see figure below). Apart from exhibiting the orange photoluminescence originating from f-f electronic transitions of Sm(III), this series of materials displays the slow relaxation of magnetization effect at low temperatures, owing to the single-ion anisotropy of a well magnetically isolated 4f metal ion. Moreover, by crystallizing in polar or chiral space groups, these materials open the perspective for adding the related physical functionalities such as piezo-, pyro-, and ferroelectricity, as well as second harmonic generation (SHG).



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Interface and Architecture Optimization in PbPc-based Organic Photodetectors

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Organic photodetectors (OPDs) are appealing candidates for medical dosimetry because of to their tissue equivalence. However, their low detection efficiency for high-energy photons hinders their use in radiology. In this work, we investigate the use of lead phthalocyanine (PbPc), a small-molecule semiconductor with optical absorption in the visible and near-infrared (NIR). The central heavy atom in PbPC can enhance X-ray attenuation when the material is used in thin-film OPDs.

The study initially focuses on interface engineering to optimize extraction and reduce recombination. The influence of different hole transport layers (HTLs), as well as their combination in bilayers, was evaluated. Injection layers such as PEDOT:PSS and molybdenum oxide (MoO_3) were also investigated, and found to reduce dark currents and overall performance parameters.

The effect of the choice of electron transport layers (ETLs) was studied as well. Materials such as C_{60}, BCP, SnO_x were evaluated as top ETLs, leading to a further improvement in efficiency. In this work we will discuss also the difference between bilayer and bulk heterojunctions (BHJ), and their implication in the design of efficient optical sensors.

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Anionic dithiolate-Au(I) complexes for the construction of luminescent heterometallic coordination assemblies

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Anionic dithiolate-Au(I) complexes have gained broad interest in materials chemistry, as they tend to organize through strong non-covalent aurophilic interactions into supramolecular moieties, leading to strong charge-transfer photoluminescence [1,2]. Moreover, as their optical properties are related to supramolecular inter- or intra-molecular interactions, their photoluminescence can be modified through changes in their structural environments, as well as the influence of external physical and chemical stimuli. Therefore, they are considered good candidates for the construction of stimuli-responsive solid luminophores employing metallophilic aggregates [3]. In our work, we focused on gold(I) iso-maleonitriledithiolate (i-mnt) complexes, $[Au^{I}_{2}(i\text{-}mnt)_2]^{2-}$, which organize into bimetallic anionic units with short aurophilic interactions, ensuring strong photoluminescence. Furthermore, their combination with other organic and inorganic cations results in the formation of coordination systems based on tunable intrametallic metallophilic interactions, which govern their optical properties. Here, we also present the results of our attempts on the combination of $[Au^{I}_{2}(i\text{-}mnt)_2]^{2-}$ ions with selected d- and f-block metal ions (Figure 1), to form heterometalic coordination systems with tunable crucial Au(I)··Au(I) interactions. The obtained materials were investigated using X-ray diffraction and spectroscopic techniques, including luminescent spectroscopy, to determine the influence of various molecular arrangements on their optical properties.

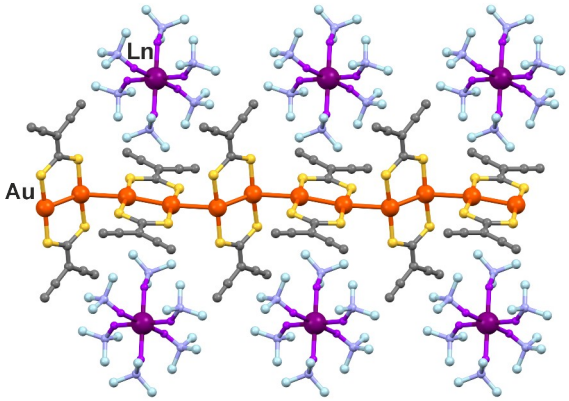

Figure 1. The crystal structure of the obtained heterometallic lanthanide(III)−gold(I) supramolecular framework incorporating photoluminescent dithiolate-gold(I) complexes.

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Ultrastable pyrazolate porphyrin metal-organic frameworks

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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 are particularly attractive for catalytic applications,[1] such as electrochemical CO_2 reduction reactions (eCO_2RR). This is thanks to their intrinsic porosity and the possibility of incorporating building blocks with high catalytic activity like metalated porphyrin linkers. However, MOF 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 eCO_2RR (**Figure 1a**). Despite the ability of pz-linkers to form topologies analogous to carboxylate ligands, examples of pz-MOFs are scarce and have seldom been tested in environmentally applications necessitating robust chemical stability.[3] Thus, we have chosen metal pz-porphyrin (pz-MP) MOFs as a platform for high-stability demanding applications. As a starting point, we have synthetized PCN-601 $[Ni_8O_6(pz\text{-}MP)_3]$[3] (**Figure 1a**) and studied its stability under eCO_2RR conditions, which at first glance is comparatively higher than equivalent porphyrin carboxylate-based MOFs (**Figure 1b**). Furthermore, as depicted in **Figure 1c**, powder X-ray diffraction (PXRD) shows that high crystallinity is maintained across all samples following exposure to a 0.5M $NaHCO_3$ aqueous solution over several days.

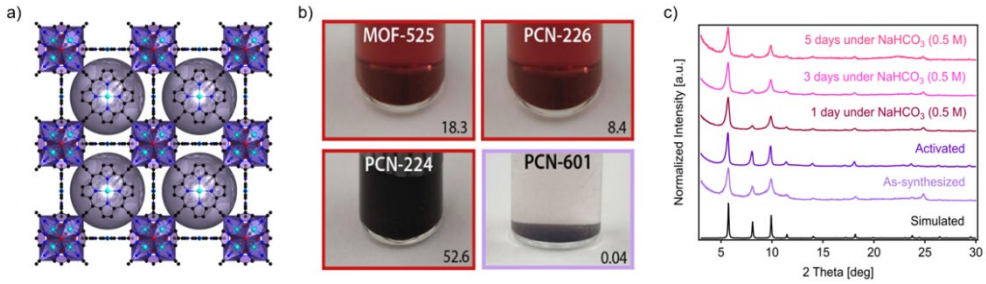

Figure 1. a. Crystal structure of MOF PCN-601.[3] **b.** Porphyrin carboxylate MOFs (red) vs porphyrin pyrazolate PCN-601 (purple) stability under $NaHCO_3$ (0.5M) buffer mimicking eCO_2RR conditions. **c.** Experimental and simulated PXRD of PCN-601 under different conditions.

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UNCONVENTIONAL PHYSICAL BEHAVIORS OF HIGHLY CORRUGATED SUPERCONDUCTING NIOBIUM THIN FILMS.

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The emerging field of *Fluxonics* includes superconducting circuitry capable of conducting and manipulating flux quanta to perform operations such as quantum computing. This technology enables the implementation of more powerful computing systems, making possible to do things like simulate new materials and drugs or develop ultra-precise sensors with very low energy consumption *[1]*. The ongoing research on fluxonics ranges from new material systems to architectures that can keep magnetic flux under control. One possible approach is shaping the superconducting systems, which permits manipulating the vortices that carry flux quanta in type II superconductors. Following this strategy, we have chosen a silicon substracte with a wavy structure comprised of a longitudinal triangular pattern that is repeated in the transversal direction *[Fig 1a].* On top of this 250 nm periodic structure we have grown a ~80nm Niobium (Nb) thin film using DC magnetron sputtering. In order to study the superconducting properties we have defined a pattern on the sample using optical lithography *[Fig 1b] to carry out electrical transport measurements under different coditions.* The objective of this project is to study how the sample behaves by varying parameters such as external magnetic field, temperature and applied current density. *[Fig 1c].*

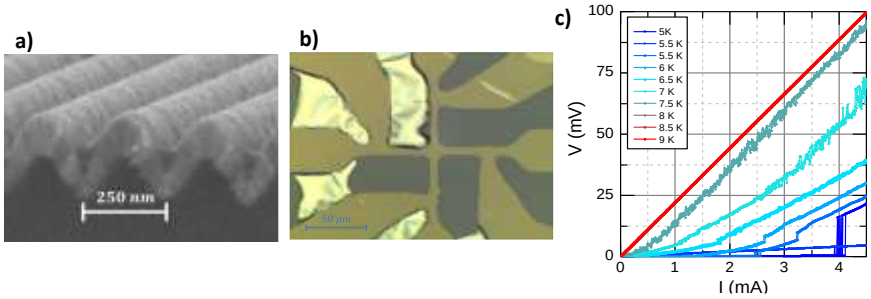

Figure 1. 1a) SEM image of the wavy structure. 1b) Optical microscopy image of the geometry used for electrical transport measurements. 1c) I-V characteristic curves for several temperatures.

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[1.1.1]propellane electrophilic activation by alkylboronates: a route to complex cyclobutanes

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The synthesis of strained carbocycles has been thoroughly studied due to its diverse applications, mainly in medicinal chemistry. The unusual orbital distribution of [1.1.1]propellane induces the formation of methylenecyclobutanes when electrophilically activated[1], by means of the energy released when breaking carbon-carbon bonds[2].

In a previous work in the group, the diborylation of [1.1.1]propellane without catalytic activation could be achieved for the first time[3], using the B-B bond in bis(catecholato)diboron (B_2cat_2) as an electrophilic reagent. In this work, we report the alkylborylation of [1.1.1]propellane using various catechol boronate esters in order to prove that another boron source could react similarly and, even more critically, create new geminal carbon-carbon and carbon-boron bonds. This methodology provides access to complex cyclobutanes that could be used as scaffolds or building blocks and otherwise would require several steps to be obtained.

Reactivity of [1.1.1]propellane

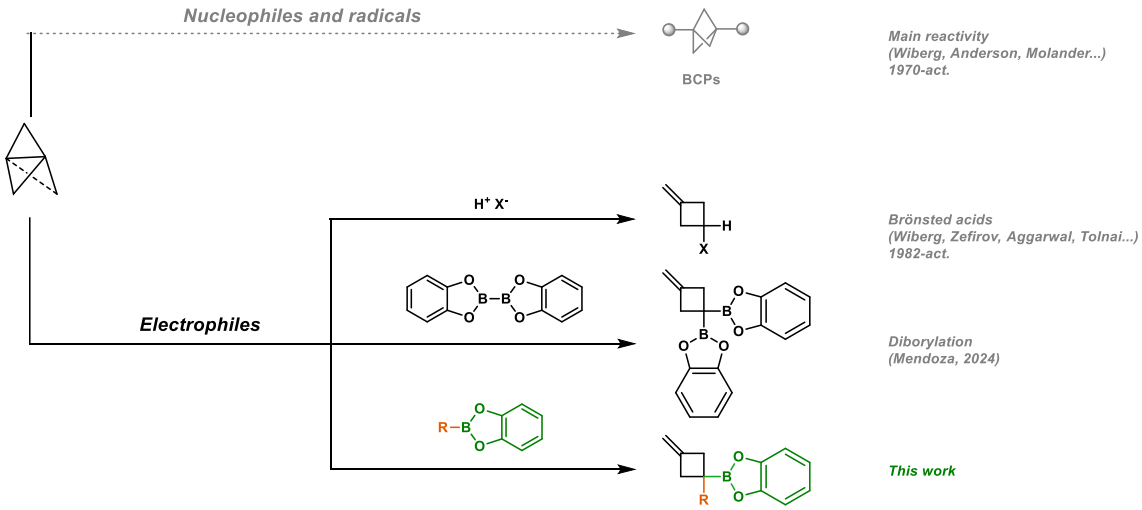

Figure 1. General reactivity of [1.1.1]propellane

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Evaporator design to tackle organic deposition speed bottle neck for Perovskite PV industrialization.

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An increasingly large number of publications, using diverse production techniques, are demonstrating the immense potential of metal halide perovskite thin-film devices.[1] Promising records in terms of power conversion efficiencies, device lifetimes and a growing library of photo-electrical applications all follow from laboratories worldwide.[2] However, these outstanding results are often obtained on a small scale, with the use of ever more complex equipment, and one of the open challenges remains to achieve commercial-scale production speeds.[3] The Molecular Opto-Electronic Device (MOED) group in Valencia has therefore chosen to focus on vacuum deposition techniques as the most promising route to perovskite application. Various works utilizing co-evaporation showed the viability of fully vacuum processed perovskite solar cells, LEDs and detectors.[1], [4] Currently multiple national and international projects focus on a wide spread of research points such as silicon-perovskite tandems, sequential evaporation and long-term solar cell stability.[5] The main focus of this talk will be on a novel route towards commercially viable deposition speeds; Gas Flow Assisted Flash Evaporation (Gas-FE). Gas-FE is a single source, rough vacuum deposition method, it easily allows for the inclusion of constituents with varying vapor pressures and is designed for large-area and extremely fast deposition. The Gas-FE has been utilized as a modestly successful single source perovskite deposition method with a promising 9.6% PCE when applied in a fully vacuum processed solar cell stack. The most attractive quality of the Gas-FE are the fast sample processing and deposition speeds of 10x10 cm^2 and over 1 µm/min while maintaining the stoichiometry of introduced the organic-inorganic perovskite powder.[6]

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Label free magnetic nanoparticles as dual nanothermometers and nanoheaters: from $CoFe_2O_4$ to Synomag

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In recent years, nanoscale systems capable of simultaneously generating and sensing heat have attracted growing interest [1]. Conventional dual-component constructs combining separate nanoheaters and fluorescent nanothermometers face major drawbacks in biological environments, including photobleaching, scattering, and biocompatibility issues.

To overcome these limitations, we previously demonstrated the label-free thermometric capability of magnetic nanoparticles (MNPs) functioning as both nanoheaters and nanothermometers. Specifically, commercial $Co_{0.3}Fe_{2.7}O_4$ nanoflowers [2] (Micromod Nanopartikels GmbH), which were employed for their efficient photothermal conversion and magnetic relaxation properties. Under 780 nm LED irradiation, heat generation was achieved, and temperature readout was performed via AC magnetometry (10–100 kHz, up to 32 kA/m), exploiting Brownian relaxation for temperature transduction [3].

In contrast, because its relaxation mechanism is Brownian, it is sensitive to even slight changes in the viscosity of the surrounding medium, leading to a reduction in its hysteresis loop. Building on this observation, we extend our approach to evaluate the potential of Synomag (Micromod Nanopartikels GmbH), a commercially available iron oxide nanoparticle, as a nanothermometer. These magnetic nanoparticles exhibit Néel relaxation, making them insensitive to variations in medium viscosity, and they have already demonstrated biocompatibility with cells.

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Green-Synthesized AuNPs from Grape Extracts: Extract-Dependent Effects on Nanoparticle Size and Sensor Performance

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Gold nanoparticles (AuNPs) are widely used in sensing applications due to their optical and electrochemical properties, however traditional synthesis methods often rely on hazardous reagents. Green synthesis using extracts derived from grapes offers a sustainable alternative to this problem. Extracts obtained from different fractions of Tempranillo grapes were evaluated as reducing and stabilizing agents for the synthesis of AuNPs, aiming to assess their suitability for electrochemical sensing applications.

Aqueous extracts from peel, seeds, juice, pulp, and whole grapes, as well as hydroalcoholic extracts (50% water–methanol) from peel and seeds, were used to synthesize nanoparticles under varying conditions of time, extract concentration, and temperature. UV–visible spectroscopy revealed consistent surface plasmon resonance peaks in the range of 530–545 nm across most samples, which indicates the formation of nanoparticles with similar sizes despite variations in synthesis parameters. These findings suggest that dominant biomolecular components within the grape extracts govern nanoparticle formation and limit size variability. Further analysis with Raman Spectroscopy and AFM provide insight into the composition of the nanoparticles.

Selected nanoparticles were incorporated into different types of electrochemical sensor platforms to evaluate their effect on sensor performance. No significant catalytic enhancement was observed under the tested conditions. Nevertheless, the results demonstrate that grape-derived extracts enable reproducible and sustainable nanoparticle synthesis. Further optimization of surface chemistry, electrode materials, and immobilization strategies may improve their applicability in sensing technologies.

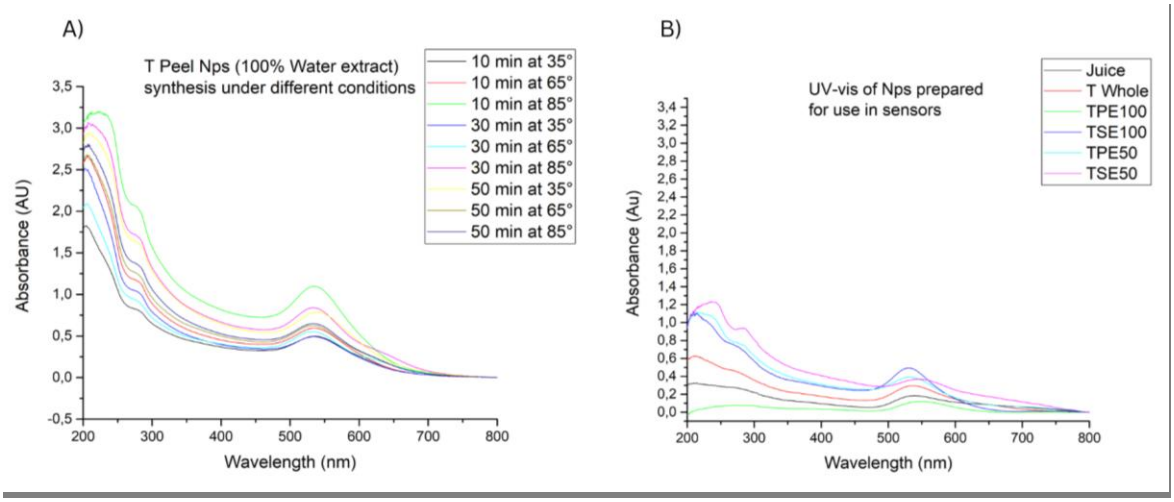

Figure 1. (A) UV–Vis spectra of gold nanoparticles synthesized from peel extract under varying temperature and reaction time conditions, showing consistent surface plasmon resonance (SPR) peaks centered around ~545 nm. (B) UV–Vis spectra of nanoparticles synthesized from different grape-derived extracts under fixed conditions (65 °C, 30 min) and a lower $HAuCl_4$:extract ratio (20:1). Although absorbance intensity varies due to concentration differences, the SPR peaks remain at similar wavelengths, indicating the formation of nanoparticles with comparable sizes across all samples.

Magnetic, hydrogen-sensing, (Fe)Pd alloy nanoparticles and their oxidation to a Pd-FeO_x core-shell structure

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Pd-based nanomaterials are widely investigated for hydrogen sensing applications [1]; however, the internal structure of bimetallic Pd systems and its impact on functional properties are often overlooked. Here, we demonstrate that exposure to ambient conditions fundamentally alters small (~4 nm), gas-phase-assembled Pd-rich Pd–Fe alloy nanoparticles (7–28 at.% Fe) by inducing Fe segregation and the formation of a Pd/FeOx core–shell structure. This conclusion is supported by a combination of structural (Figure 1a), spectroscopic, magnetic, and hydrogen absorption measurements (Figure 1b) performed on highly porous films (Figure 1c) composed of surfactant-free nanoparticles. We show that Fe segregation proceeds via a nanoscale Kirkendall-type mechanism, involving outward diffusion of Fe and subsequent oxidation at the nanoparticle surface. This process leads to the formation of ultrathin (<1 nm), amorphous FeOx shells, which give rise to glassy magnetic behavior. Importantly, we demonstrate that segregation and oxidation can be suppressed by embedding the nanoparticles in a metallic Nb matrix, resulting in continuous nanogranular films that exhibit conventional superparamagnetic blocking consistent with moderately dilute dispersions of ferromagnetic Pd–Fe nanoparticles. Electrical resistance measurements under cyclic hydrogen exposure reveal an irreversible decaying background in porous oxidized films, which we attribute to the progressive reduction of surface Fe oxide, further supporting the proposed core–shell morphology. These results highlight oxidation-driven segregation as a key mechanism governing the magnetic and hydrogen-sensing properties of Pd–Fe nanoparticles.

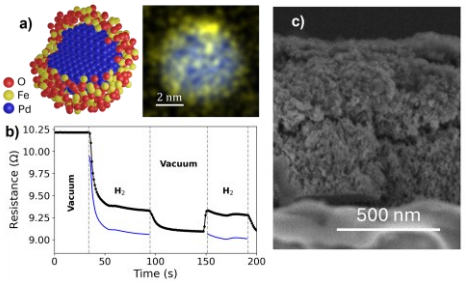

Figure 1. a) Micro-EDX analysis of an FePd nanoparticle showing Fe segregation toward the surface and the formation of a Pd-rich core. b) Electrical resistance response of a nanoparticle film with 26 at.% Fe, showing its time evolution under alternating vacuum conditions (0.045 mbar) and atmospheric-pressure Ar + 5% H_2. c) Cross-sectional SEM image of a highly porous nanoparticle film.

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