ICMOL

Activity Report
2020-2023

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ICMOL | Universitat de València | Excelencia María de Maeztu 2020- 2024

2020-2023

ICMOL

INSTITUTE OF
MOLECULAR SCIENCE
UNIVERSITAT DE VALÈNCIA

Contents

Message from the Director

Eugenio Coronado
Director of ICMol

It has been over two decades since the creation of ICMol in the year 2000, and it's time to reflect on the journey without succumbing to complacency or nostalgia. In the realm of fundamental research, it's crucial to look ahead, identify the frontiers of knowledge, and actively explore them. This perspective holds particular significance for those involved in the leadership and management of research centers like ICMol.

It is part of our mission at ICMol, to continue advancing the role of molecular aspects of nanoscience and new materials, achieving the grand technological challenges of our global society. Let's say, exploring small matter for a better life.

That was our goal when we created this center in 2000. Just 15 years later, the ICMol achieved recognition as a Maria de Maeztu Unit of Excellence by the Ministry of Science and Innovation due to the prestige accumulated by our multidisciplinary research groups.

This continues today. Our researchers gather grants and awards from the highest research institutions, such as the European Research Council, and their articles are widely cited in scientific journals.

The Master in Molecular Nanoscience and Nanotechnology (interuniversity) as well as the Master's in Theoretical Chemistry and Computational Modeling, along with their associated courses and doctoral programs, are highly sought after. Additionally, ICMol plays a significant role in organizing the European School of Molecular Nanoscience (ESMolNA), a training school aimed at providing a suitable framework for showcasing and extensively discussing the state of the art.

We are on the frontline in raising funding from national and European institutions. We maintain a strong commitment to industry to boost collaborative projects to help companies to be more competitive and to make advances towards sustainability.

Since 2018, the Generalitat Valenciana promotes ICMol's Scientific Unit for Industrial Innovation (UCIE) to facilitate transfer to industry. We have built a reservoir of knowledge that companies can use to solve the problems they face.

Through pioneering research and broad-based education, at ICMol we will continue to strengthen our international reputation for excellence in molecular materials solutions to future challenges in health, sustainability, energy efficiency, national security, and advanced manufacturing. Our vision is to remain pioneers in this molecular approach.
Hope you find the site useful.

Welcome to ICMol.

Small Matter for a better life

EL PAÍS, sábado 2 de diciembre de 2000

CIENCIA ▶ APUESTA PIONERA DE LA UNIVERSIDAD DE VALENCIA

El Instituto de Ciencia Molecular unifica la investigación en este área

Será el primer centro de ciencia molecular

La Universitat presenta un instituto para investigar y diseñar nuevos materiales

ICMol approval: July 25, 2000 - Building inauguration: December 12, 2005

Organization and structure of the institute

ICMol is a research institute of the University of Valencia (UV) founded in 2000 to develop a competitive and high-quality research in materials science using a molecular approach. ICMol's governance structure is made up of the following persons who head the management staff:

Scientific Director: Professor Eugenio Coronado

Garantees Council (2020-2023): Henk Bolink, Enrique Ortí, Guillermo Mínguez-Espallargas, Alejandro Gaita-Ariño, Carlos Martí-Gastaldo, Efrén Navarro-Moratalla, Emilio Pardo, Gonzalo Abellán.

GOVERNING BOARD

ICMol is the sole university institute at the Valencia community accredited as Unit of Excellence Maria de Maeztu. In this frame, ICMol has created a Governing Board formed by the Scientific Director and the Garantees for decision making, priority setting and management of the research (Strategic Lines) and educational activities (two masters and doctorate programs coordinated by the ICMol).

ICMol has sharply improved the management of the center creating various structures that provide technical and organisational support, namely:

1) The Research Management Unit, coordinated by a Project Manager, that is in charge of the execution and justification of the Maria de Maeztu grant, the application and management of infrastructure grants, and of providing general support and advice for project application and management.

2) The Education Unit, in charge of managing the educational and training activities, including the organization of scientific events, schools, workshops, master and doctorate programs.

3) The Knowledge Transfer and Communication Units, coordinated by an Executive Manager, who is also in charge of a Unit of Technical support that maintains the common infrastructure of the center. With a communication officer for enhancing ICMol's visibility and reinforcing the strategic areas.

SCIENTIFIC ADVISORY BOARD (SAB)

The SAB is composed by 6 internationally renowned experts in the different scientific areas, covering the complete spectrum of topics in which the research at ICMol focuses. The SAB members are:

Prof. Neil Champness, Norman Haworth Professor of Chemistry, began his academic career at the University of Southampton, obtaining his B.Sc. (1989) and PhD (1993). He took up his current position at the University of Birmingham in 2021.

Prof. Rene Janssen, Director of the interdepartmental research group Molecular Materials and Nanosystems at Eindhoven University of Technology. His expertise includes the Chemistry and Material Science for optoelectronic molecular devices.

Prof. Bettina V. Lotsch, Director at the Max Planck Institute for Solid State Research in Stuttgart. Her expertise includes new materials for energy conversion and storage, photonic nanostructures for optical sensing and 2D nanosheet materials and artificial heterostructures.

Prof. Maurizio Prato, Carbon Nanobiotechnology Group Leader at CIC biomaGUNE in San Sebastián. His expertise includes the Chemistry and Materials Science of carbon nanostructures and their biomedical applications.

Prof. Ángel Rubio, Director of the Theory Department of the Max Plank Institute for Structure and Dynamics of Matter at Hamburg. His expertise includes the theory of materials with electrical, magnetic and optical properties.

Prof. Roberta Sessoli, Professor of General and Inorganic Chemistry in the Department of Chemistry at the University of Florence. Her expertise includes molecular magnetism, quantum technologies and spintronics.

COMMITTEE FOR GENDER EQUALITY

Finally, ICMol is engaged in gender issues and a Committee for Gender Equality has been formed (Equipo Igualdad ICMol). This Committee is in charge of the organization of Gender and Diversity Events (11 of February workshops and March 8th Conference).

This management structure has shown to be very efficient in organizing and coordinating the different activities of the center. It is worth to mention that the Communication Unit has been created in this last period and is strongly enhancing the local and international visibility of the ICMol at different levels (scientific, industrial, outreach, social).

RESEARCH GROUPS

Owing to its remarkable growth during the last years, ICMol's current structure is slightly different to the original with a total of 17 research groups, where the new ones are led by emerging researchers launching their own research lines (European Research Council grantees).

Groups

- Research Team on Molecular Materials (RTMM)
- Theoretical Chemistry Group (MolMatTC)
- Coordination Chemistry Group (CCG)
- Switchable Molecular Materials Group (SMMG)
- Supramolecular Chemistry Group (SCG)
- Quantum Chemistry of the Excited State Group (QCEXVAl)
- Photochemistry Reactivity Group (PRG)
- Solid State Spectroscopy Group (SSSG)
- Sustainable Organic Chemistry Group (SOC)
- Membrane Biophysics Group (MBP)
- Molecular Optoelectronic Devices Team (MOED)
- Functional Inorganic Materials Team (FUNIMAT)
- Crystalline Inorganic Solids Lab (CRISOL)
- Multifunctional Porous Materials (MUPOMAT)
- Crystal Engineering Lab (CEL)
- Two-Dimensional Materials Chemistry Lab (2DChem)
- 2D Smart Materials Lab (2DSmartMat)

Groups by lines

Line 1: Metal-Organic Frameworks (MOFs)

- Switchable Molecular Materials Group
- Functional Inorganic Materials Team
- Multifunctional Porous Materials
- Research Team on Molecular Materials

Line 2: 2D Materials

- Research Team on Molecular Materials
- Solid State Spectroscopy Group
- Crystalline Inorganic Solids Lab
- Crystal Engineering Lab
- Two-Dimensional Materials Chemistry Lab
- 2D Smart Materials Lab

Line 3: Molecular design of biomaterials

- Supramolecular Chemistry Group
- Quantum Chemistry of the Excited State Group
- Membrane Biophysics Group
- Functional Inorganic Materials Team
- Quantum Chemistry of the Excited State Group

Line 4: Molecular spintronic devices

- Research Team on Molecular Materials
- Coordination Chemistry Group
- Switchable Molecular Materials Group

Line 5: Molecular Spins for Quantum Technologies

- Research Team on Molecular Materials
- Coordination Chemistry Group

Line 6: Molecular Electronic Devices

- Molecular Optoelectronic Devices Team
- Theoretical Chemistry Group
- Photochemistry Reactivity Group
- Research Team on Molecular Materials

2023

A center of excellence in Molecular Nanoscience

- Management of the European Institute of Molecular Magnetism
- **Research projects of excellence:**

European projects active during this period
20 European Projects (of which 9 ERC Grants)

NATIONAL /
María de Maeztu Unit of Excellence

A center of excellence in chemistry and materials science

In Chemistry more than 90% of the high impact publications of the Univ.Valencia are generated by the ICMol (source: web of Science).

A European Center for Higher Education

- Master and PhD Program in Nanoscience and Molecular Nanotechnology
- Master and PhD Program in Theoretical and Computational Chemistry (ERASMUS-MUNDUS)

NUMBERS

175 Scientific publications

9 ERCs Active

17 Research Groups

88 Theses Current

2 European Doctoral Networks

2 Spin offs

2023

Members

- **11 Full Professors**
- **20 Associate Professors**
- **11 Ramón y Cajal Researchers**
- **12 Postdocs Juan de la Cierva and Marie Curie**
- **26 Postdocs + 62 Predocs**
- **38 Technicians and Support Staff**
- **23 Master's students**

203 ♂ 121 ♀ 82

25 countries

2 Research Lines

LINE 1. METAL-ORGANIC FRAMEWORKS

1. Introduction

The specific research objectives and priorities of Line 1 are:

O1.1) Mesoporous flexible MOFs. We proposed to investigate the rare breathing phenomenon occurring in MOFs in order to tune the physical properties upon structural changes. Furthermore, the inclusion of functional molecules in the channels of the framework can give rise to hybrid functional MOFs combining an extended lattice with a molecular lattice, providing an ideal platform to create new multifunctional materials covering from the simple coexistence of different properties to a synergy between these functionalities.

O1.2) Electrically conductive MOFs. MOFs that exhibit both high surface area and electrical conductivity constitute one of the open challenges in this area. They are emerging as a new class of materials whose applications reach beyond those typical of porous solids, including supercapacitors, chemiresistive sensing, field-effect transistors or thermoelectrics, among others. We proposed to prepare electrically conductive MOFs and investigate their processing in order to incorporate these materials into devices.

O1.3) Catalytically-active metal species hosted in MOFs. These porous materials have already shown a unique host-guest chemistry, being suitable candidates to encapsulate and stabilize highly active but highly unstable metal species within the pores. Moreover, recent works have demonstrated that MOFs can be used as effective chemical nanoreactors to construct, in-situ, original metal species difficult to obtain outside the pores that are efficiently retained and stabilized showing outstanding catalytic activities. We pretended to go one step further by synthesizing subnanometer metal clusters and supramolecular coordination compounds within MOFs, capable to compete with industrial catalysts.

O1.4) MOFs for environmental remediation. Contamination of aquatic environments is one of the major concerns of todays society. Thus, the design of novel materials capable to selectively remove contaminants from water are mandatory. MOFs are porous materials featuring channels of controllable size, shape and a proper functionality. We planned to develop novel families of water-stable highly robust MOFs whose empty space is accordingly designed to capture contaminants efficiently, selectively and reversibly.

2. Highlights

Porous molecular materials with conductive or magnetic properties

We have combined porosity and conductivity in a molecular material via the development of semiconductor porous hydrogen-bonded organic frameworks (HOFs). In particular, by tuning the synthetic conditions a zwitterionic tetrathiafulvalene derivative is obtained, with a positively charged TTF core and a negatively charged carboxylate group, with an efficient charge transport with no need for postsynthetic treatment (e.g., electrochemical oxidation or doping). Open structures (ca. 20 % volume) with CO_2 sorption capacity of ca. 2 mmol g^{-1} and record experimental conductivities of 1.35×10^{-6} S cm^{-1} are achieved (see Figure 1), which can be easily processed as thin films due to their facile solubility.[1]

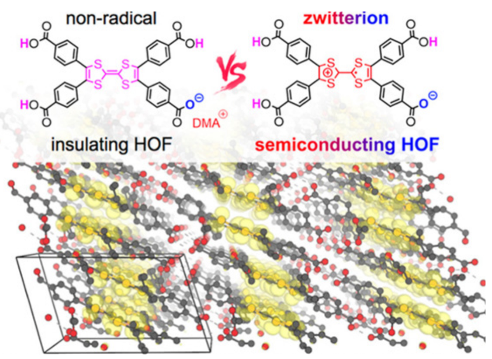

Figure 1. Zwitterionic approach to obtain a semiconductive HOF.

Furthermore, we have been able to prepare a MOF-carbon nanotube composite displaying porosity, conductivity and stability by decorating the surface of single-crystals of a tetrazine-based MOFs with an ultrathing coating of single-wall carbon nanotubes, in one step, resulting in conductivity values of $4x10^{-2}$ S cm^{-1} at room temperature.[2]

At ICMol we have also pioneered the design of MOF magnetic materials. A key result in this period has been the report of layered MOFs showing tunable magnetic properties. These van der Waals materials can be exfoliated down to the monolayer and magnetically characterized via mechanical measurements when integrated in a membrane-type structure. These results are described in detail in line 2 (2D materials).

Catalysis

MOFs have shown a unique capability to promote reactions and stabilize unstable metal species within the pores. In this sense, we have developed the gram-scale preparation and stabilization of Pd single-atom catalysts (SACs) within the functional channels of a novel methyl-cysteine-based MOF, resulting in a robust and crystalline solid catalyst that allows its implementation in industrially viable conditions, which are difficult to achieve due to the requirement of particular conditions and supports for their synthesis, together with the need of solvents and additives.[3]

We have also managed to incorporate Pd(II) metal centres into the framework of a highly robust MOF with a solvent-assisted reaction using a Pd-metalloligand. We have established its activity, selectivity and recyclability in the the Suzuki–Miyaura allylation of aryl and alkyl boronates, demonstrating that this material acts as an efficient heterogeneous catalyst for the C–C bond formation between a range of alkyl, aryl and alkenyl boronates with different allyl bromides.[4] Other subnanometer metal clusters such as Ag^0_2 and Fe^{3+} single atoms have also been successfully isolated withing the channels of a MOF, resulting in a material capable of catalyzing the unprecedented direct conversion of styrene to phenylacetylene in one pot.[5]

We have also shown that an amino acid-derived MOF, densely decorated with alcohol–containing arms and adsorbed water, enables selective hydrolysis of glycosyl bonds. The supramolecular order with the so–formed chiral fragments allows the absolute determination of the organic structure by single–crystal X–ray crystallography, all in a single operation (see Figure 2). This is analogous to retaining hydrolase enzymes, but without the participation of formal protons, with the advantage of being capable of determining the absolute structural determination of the natural product by single–crystal X–ray crystallography.[6]

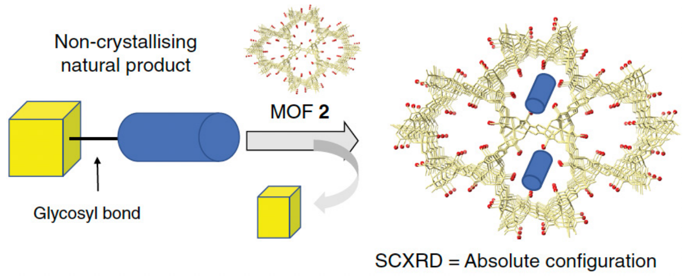

Figure 2. Schematic representation of the one-pot selective hydrolysis/adsorption/crystal resolution of a natural product within a MOF.

We have used solvent-assisted linker exchange reactions to produce a family of UiO-68 derivatives in which a photoactive tetrazine-based ligand can be incorporated in a controlled manner as a uniform mixture or the formation of core–shell domains (see Figure 3), having drastic changes in the photocatalytic activity toward proton or methyl viologen reduction. This behaviour is unique of the multivariate framework, as the analysis of the single linker phases reveals the necessity of combining both linkers to combine efficient light sensitization, chemical stability, and porosity, all relevant to photocatalysis.[7]

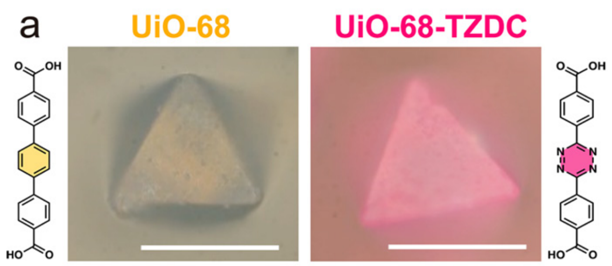

Figure 3. (Left) size and morphology of UiO-68. Scale bars correspond to 50 μm. (Right) size and morphology of photoactive UiO-68-TZDC crystals. Scale bars correspond to 25 μm.

We have also decribed the preparation of an heterometallic TiFe2 cluster-based MOF that combines Lewis Ti^{4+} and Brønsted Fe^{3+}–OH acid sites, which has been applied to the synthesis of β-amino alcohols with a scope that also includes the gram scale synthesis of propranolol, a natural β-blocker listed as an essential medicine by the World Health Organization, with excellent yield and selectivity.[8]

MOFs for environmetal issues

We have described a new synthetic protocol that allows the synthesis of highly active and stable catalysts, based on abundant elements, for the direct transformation of CO_2 to carbon monoxide, one of the most important chemical building blocks. This has been achieved by the thermal decomposition of the heterometallic MOF MUV-101(Fe, Ti), resulting in the formation of carbon-supported titanomaghemite nanoparticles (see Figure 4) that display outstanding catalytic activity for the production of CO from CO_2 via the reverse water-gas shift (RWGS) reaction with CO selectivity values of ca. 100% and no signs of deactivation after several days on stream.[9]

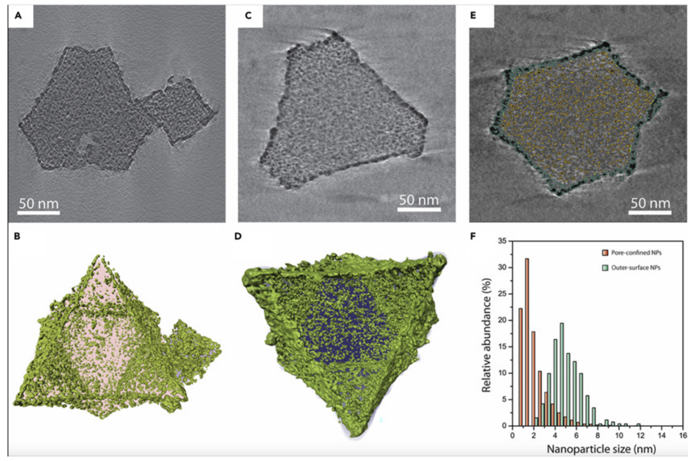

Figure 4. Electron tomography analysis of the TiFe/C catalyst.

In the same line, we have reported an anilato-based MOF containing triazole linkers as substituents that presents a 3D microporous structure with voids with a high affinity for CO_2 molecules and small channels that enable the selective entrance of CO_2 but not of molecules with larger kinetic diameter such as N_2 or CH_4. This novel MOF has shown to be useful for CO_2 uptake and separation, with particular attention to CO_2/N_2 and CO_2/CH_4 gas mixtures. Breakthrough experiments have provided direct experimental evidence of the capacities of this MOF for selective sorption of CO_2 vs N_2 or CH_4, with excellent selectivities that place it among the best porous coordination polymers / metal-organic frameworks for these separations. In addition, regeneration of the material is easily achieved at mild conditions, simply by flowing argon with no need of increasing temperature.[10] Furthermore, we have investigated the CO_2:N_2 separation performance of a hydrophobic MOF presenting open-metal sites under extremely humid conditions, an essential condition given that water vapor is inevitable among most industrial flue gas mixtures. The carborane-based MOF presents competitive capacity and remarkable selectivity

Research Lines

values for carbon dioxide adsorption in CO_2:N_2 mixtures, and also stands for its excellent water stability along the separation process.[11]

We have also investigated the use of a novel MOF derived from the amino acid S-methyl-L-cysteine in mercury removal using mixed matrix membranes (MMMs). These MOF-based MMMs exhibit high efficiency and selectivity—in both static and dynamic regimes—in the removal of Hg^{2+} from aqueous environments, due to the high density of thioalkyl groups decorating MOF channels (see Figure 5). These MMMs are capable to reduce different concentration of the pollutant to acceptable limits for drinking water (<2 parts per billion), and a novel device, consisting of the recirculation and adsorption of contaminated solutions through the MOF–MMMs, has been designed and successfully explored in the selective capture of Hg^{2+}.[12] Multivariate MOFs based on combinations of aminoacids have also proved to be very efficient for the capture of antibiotics from environmental matrices.[13] In particular, we have reported a a family of three isoreticular MOFs, derived from natural amino acids, that exhibit high efficiency in the removal of a mixture of four distinct families of antibiotics, such as fluoroquinolones, penicillins, lincomycins, and cephalosporins, as solid-phase extraction (SPE) sorbents.

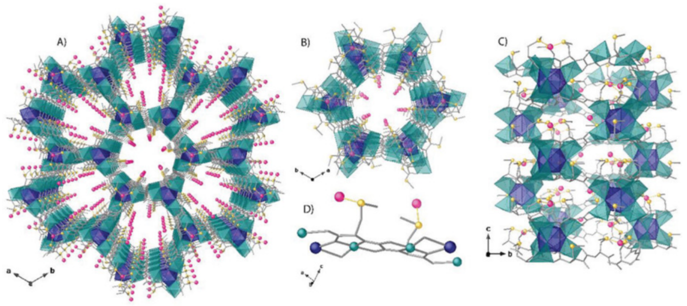

Figure 5. Crystal structure of a MOF incorporating $HgCl_2$ in the pores.

Titanium-based MOFs

We have described an unprecedented methodology for the synthesis of heterometallic titanium frameworks by metal-exchange reactions of MOF crystals at temperatures below those conventionally used in solvothermal synthesis. The combination of hard (titanium) and soft (calcium) metals in the heterometallic nodes of MUV-10(Ca) enables controlled metal exchange in soft positions for the generation of heterometallic secondary building units (SBUs) with variable nuclearity, controlled by the metal incorporated (see Figure 6). The structural information encoded in the newly formed SBUs drives an MOF-to-MOF conversion into bipartite nets compatible with the connectivity of the organic linker originally present in the crystal. In comparison to de novo synthesis, this metal-induced topological transformation provides control over the formation of hierarchical micro-/mesopore structures at different reaction times and enables the formation of heterometallic titanium MOFs not accessible under solvothermal conditions at high temperature, thus opening the door for the isolation of additional titanium heterometallic phases not linked exclusively to trimesate linkers.[14] In addition, the different affinity of Ti(IV) and Ca(II) sites was used to direct selective coordination of amines. This enables the combination of Lewis acid and available -NH_2 sites in sizeable pores for cooperative cycloaddition of CO_2 to epoxides, with full conversion of propylene oxide at room temperature and atmospheric pressure in absence of additional co-catalysts and with excellent cyclability.[15]

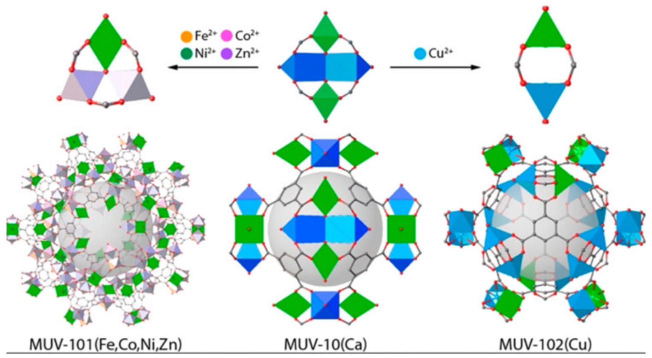

Figure 6. Metal exchange reactions with MUV-10(Ca) crystals.

We have also explored the formation of titainium-organic polyhedra. Metal–organic polyhedra (MOPs) consist of metal centers and organic linkers—similar to metal–organic frameworks (MOFs), but MOPs are molecular in nature instead of forming extended porous solids. They could be useful, e.g., when integrated into membranes. However, it is challenging to prepare MOPs that remain stable and porous after guest molecules are removed. A key result has been the report of the first titanium–organic polyhedra, $[Ti_8(p\text{-}H_2bdha)_8(p\text{-}bdha)_4]$ (cMUV-11), displaying permanent porosity (BET surface area of 1020 $m^2\ g^{-1}$) and the possibility to functionalize the ligands to tailor the properties of the MOP.[16]

Growth control of MOFs

In MOF synthesis, the mechanisms and pathways underlying their formation remain largely undisclosed. a collaboration with the group of J. Puigmartí-Luis at ETH Zurich has demonstrated that diffusion-controlled mixing of reagents at the very early stages of the crystallization process (i.e., within ≈40 ms), achieved by using continuous-flow microfluidic devices, can be used to enable novel crystallization pathways of a prototypical spin-crossover MOF towards its thermodynamic product (see Figure 7). In particular, two distinct and unprecedented nucleation-growth pathways were experimentally observed when crystallization was triggered under microfluidic mixing. Full-atom molecular dynamics simulations also confirm the occurrence of these two distinct pathways during crystal growth. In sharp contrast, a crystallization by particle attachment was observed under bulk (turbulent) mixing. These unprecedented results provide a sound basis for understanding the growth of CPs and open up new avenues for the engineering of porous materials by using out-of-equilibrium conditions.[17]

Research Lines

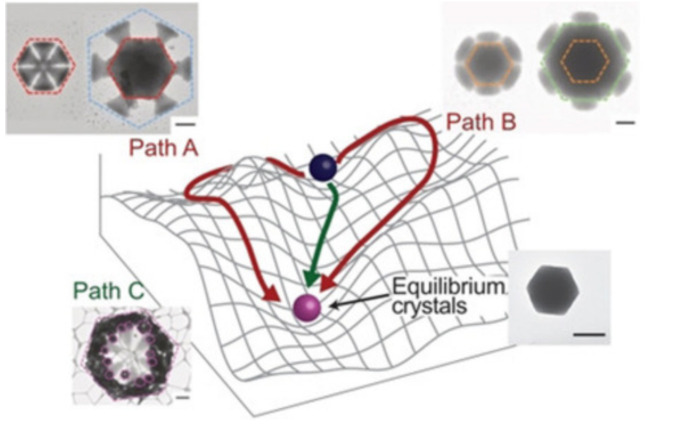

Figure 7. Different crystallization pathways depending on the mixing protocol.

3. Outlook

The research line "Metal-Organic Frameworks" has been extremely prolific in the "Maria de Maeztu" project. Different synthetic approaches have been developed, independently, mainly by 3 experimental groups (Pardo, Mínguez-Espallargas and Martí-Gastaldo) within the frames of their ERC projects in which novel porous materials have been prepared for several applications, including conductivity, magnetism, catalysis, gas separation and water remediation. We have also generated mesoporous systems through the incorporation of defects, and investigated the mechanisms of crystal growth on two different MOFs. Finally, we have also started to study two different types of molecule-based porous solids: metal-organic polyhedra (MOPs) and hydrogen-bonded organic frameworks (HOFs). To perform this work, we have extensively collaborated with theoretical groups in the modelling of different physical and chemical properties and their correlation with the structure, and established close links with national and international partners.

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LINE 2. 2D MATERIALS

1. Introduction

The specific research objectives and priorities of Line 2 are:

O2.1) 2D Physics: spin textures and tunable superconductivity at the 2D limit: 2D magnetic materials, including magnets, materials with non-colinear magnetism, quantum spin liquid candidates; 2D superconductors, including twisted monolayers of superconductors.

O2.2) 2D Chemistry: development of the chemistry and processing of novel 2D materials beyond graphene: i) layered elemental 2D pnictogens: P, As, Sb and Bi.; ii) 2D layered coordination polymers / MOFs exhibiting magnetic functionality; iii) Anionic 2D materials based on layered hydroxides as building blocks of architectures for energy storage and conversion, proton membranes and sensing.

O2.3) Design of stimuli-responsive mhybrid heterostructures with tunable properties.

2. Highlights

Vertical transport across atomically thin 1T-TaS_2

1T-TaS_2 exhibits a multifaceted electronic and magnetic scenario due to the existence of several charge density wave (CDW) configurations coexisting with exotic quantum spin liquid (QSL) states, which are highly dependent on the out-of-plane stacking of the CDW. In this work, atomically-thin layers of 1T-TaS_2 are integrated between a few graphene layers and their electrical transport properties are measured. A progressive transition is detected with different activation energies between 200 K and 70 K, and a gap in the few layer limit. These results are supported by DFT+U calculations, highlighting the confinement of electrons across the layers when approaching the 2D limit.[1]

Van Der Waals Heterostructures Based on Atomically Thin Superconductors

In this work, we report the fabrication and electrical transport characterization of vertical van der Waals heterostructures based on atomically thin layers of various TaS_2 polytypes, with semiconducting or metallic properties, between superconducting $NbSe_2$ layers. This approach represents a proof of concept of the assembly of strongly correlated low-dimensional materials between 2D superconductors and opens the door to further studies involving 2D magnets or topological insulators as barriers.[2]

Understanding magnetism in 2D: theory and magnetic force microscopy in magnetic 2D materials

The isolation of the first free-standing hysteretic magnetic 2D material, CrI3, in 2017 marked the beginning of a new field that unveiled both new physics and new opportunities for applications in magnetic devices. This discovery also sparked an increasing interest in the investigation of the fundamental physics of spin interactions at the ultimate limit of few-atom-thick materials. Indeed, the development of applications in real technologies requires a deep understanding of their magnetic properties., for instance, by employing archetypal spin models, such as Ising or Heisenberg. This gives a guide to what kind of magnetic behaviour is to be expected in a potential device. Although CrI3 has been assigned as an Ising ferromagnet, recent findings indicate that its magnetic properties are far beyond Ising. Higher-order exchange interactions and quantum effects are widely known to play an important role in describing the properties of low-dimensional magnetic materials.

In this work, we perform a combined experimental (joint effort of two groups at ICMol) and theory (in collaboration with the group of Elton G. Santos, Queens University Belfast) effort to understand the magnetism of 2D material CrI3. We identify the need for a more complex spin model. Thus, we used a suite of magneto-optical Kerr effect microscopy, magnetic force microscopy, correlated first-principles methods and Monte Carlo techniques including higher-order exchange interactions, to identify CrI3 as a quantum non-Heisenberg material. We find that biquadratic exchange interactions are essential to quantitatively describe the magnetism of CrI3 but requiring quantum rescaling corrections to reproduce its thermal properties. The quantization of spin-wave excitations at the low temperature regime is reflected on the fluctuations of the magnetization which follows Bose-Einstein rather than the Boltzmann statistics. These fluctuations induce the formation of metastable magnetic domains stabilizing into a single macroscopic magnetization or even monodomains over large surface areas (e.g. several µm's). Such domains display hybrid characteristics of Néel and Bloch types with a narrow domain wall width in the range of 3-5 nm. Similar behaviour is expected for the majority of 2D vdW magnets where higher-order exchange interactions are appreciable.[3]

Unravelling the magneto-structural phase diagram of magnetic 2D materials

In this work we unveil the phase diagram of CrI_3 over a wide range of varying temperatures. We discovered that the traditionally identified Curie temperature of bulk CrI_3 at 61 K does not correspond to the long-range order in the full volume (VM) of the crystal but rather a partial transition with less than ~25% of VM being magnetically spin-ordered. This transition is composed of highly disordered domains with the easy-axis component of the magnetization (S_z) not being fully spin-polarized but disordered by in-plane components (S_x, S_y) over the entire layer. As the system cools down, two additional phase transitions at 50 K and 25 K drive the system to 80% and nearly 100% of the magnetically ordered volume, respectively, where the ferromagnetic ground state has a marked Sz character yet also displaying finite contributions of S_x and S_y to the total magnetization. Each transition has its own characteristics in terms of magnetic ordering, thermal disorder and volume-wise electronic phases. Such complex magnetic structure is typically only seen in cuprates, iron-based superconductors, ruthenates, topological kagome magnets and manganites (see Introduction for references). For such materials the interplay between different electronic and magnetic factors plays an important role including chemical composition, geometry and electron-electron interactions. Nevertheless, we found that this is not the case for CrI_3. We used a complementary suite of several experimental techniques (µSR spectroscopy, SQUID) and theoretical approaches (correlated first-principles methods and Monte Carlo simulations including higher-order exchange interactions) to portray the phase-diagram of CrI_3 and undoubtedly reveal its competing magnetic phases.

Magnetism in layered materials is a hot area of research for the condensed matter community. Our results suggest that not only CrI_3 shows such a lower temperature for full spin-polarization of the crystal but every magnetic material that can be exfoliated to thin layers and potentially grown on a substrate as individual monolayers. This clearly raises several interesting questions, such as what the effect of competing magnetic phases in storage media? and/or are 2D magnets really feasible for implementation in real device technologies since the threshold temperature is much lower than the Curie temperature? In addition, we report, to the best of our knowledge, the first phase-diagram of 2D van der Waals (vdW) CrI_3 magnet as function of temperature based on muon spin relaxation-rotation (µSR) spectroscopy, which showed a rich set of competing magnetic phases not ever observed before.[4]

Tuning the magnetic properties and topology of 2D magnetic MOFs by chemical design

This work at the intersection between the fields of molecular magnetism, MOFs and 2D materials, exploits the chemical design of layered magnetic coordination polymers based on benzimidazole derivatives to produce novel 2D molecular-based magnets with novel topologies and tunable magnetic properties using a solvent-free synthetic route. By modifying the organic part (from monosubstituted to disubstituted benzimidazole), it has been possible to change the crystal structure and the magnetic topology from a square lattice to a distorted hexagonal one (Figure 1). [5]

Interestingly, the very weak van der Waals forces between the layers has allowed us to isolate atomically thin layers of micrometer size flakes using a micromechanical exfoliation method. This result can be highly relevant in the field of 2D materials: First, it can offer an alternative way to that provided by solid-state chemistry for the preparation of robust 2D magnets. In fact, the coordination chemistry approach has afforded the isolation of 2D magnetic materials relatively stable in open air, in sharp contrast to the few reported examples of 2D inorganic magnets. Second, the chemical versatility of the method allows novel magnetic topologies to be obtained in two dimensions.

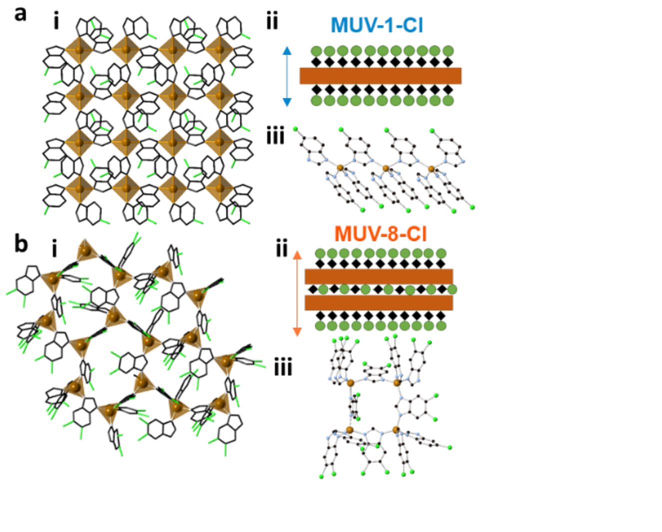

Figure 1. 2D magnetic MOFs based on benzimidazole-type ligands coordinated to Fe(II); a) MUV-1-Cl: Structure of a single layer obtained from Cl-monosubstituted benzimidazole ligands; b) MUV-8-Cl: Structure of a double layer obtained from Cl-disubstituted benzimidazole ligands.

The most relevant result in this context has been the isolation of a double layer antiferromagnet exhibiting an unprecedented topology, which is based on the assembly of two hexagonal monolayers through coordination bonds. Third, the exfoliated thin layers have been used as nanomechanical resonators, thus enabling the detection of the magnetic ordering in these antiferromagnetic thin layer systems. This mechanical detection of the magnetic ordering in a 2D antiferromagnet is novel and very powerful since it opens an efficient and general way to sense phase transitions in 2D materials in the 2D limit. [6]

Chemistry of antimonene

A new synthetic methodology using a colloidal chemistry approach has allowed the large-scale preparation of antimonene nanosheets with excellent morphological and structural quality. These results open the door for the development of heavy pnictogens-based technologies since it allows for the first time the large-scale synthesis of high-quality nanosheets for applications in electronics, biomedicine or energy storage and conversion, to name a few. In , this context, we have investigated the oxidation of liquid-phase exfoliated antimonene nanosheets and its consequences on the preparation of electronic devices and electrode contacts. [7,8]

Quantifying the Covalent Functionalization of Black Phosphorus

In this paper, we carried out for the first time the chemical reductive covalent functionalization of thin-layer black phosphorus (BP) using different BP intercalation compounds. Importantly, this work revealed the lattice opening (i.e. P–P bond breakage) of the BP structure after the functionalization. Moreover, we discovered that by changing the alkali metal concentration it is possible to tune the functionalization degree. Moreover, the first Raman spectroscopic quantification of the functionalization degree in phosphorene has been carried out, thus opening the door for the straightforward characterization of the covalent functionalization in this sort of 2D materials. These results demonstrated the great level of chemical control achieved with phosphorene paving the way for the development of electronic devices with heavy pnictogens (Sb and Bi). [9]

Potassium Intercalation and Reductive Covalent Functionalization of Carbon Nano-Onions

Multishell fullerenes, i.e., nanostructure composed of fullerenes of different sizes in a concentric arrangement, are also called carbon nano-onions. They have promising applications in energy conversion and storage. They can be functionalized covalently; however, their low reactivity led to very low functionalization degrees. Herein, we deciphered for the first time the intercalation of alkali metals between the concentric graphene layers by using vapor-phase intercalation. Raman spectroscopy showed a Fano resonance, characteristic for highly doped potassium-intercalated compounds. Moreover, these intercalated nanocarbons were covalently functionalized using n-hexyl iodide or phenyl iodide. Overall, this work could be useful for the design and synthesis of carbon nano-onions for applications in energy storage or biomedicine, to name a few.[10]

Stimuli-responsive hybrid heterostructures: Spin-crossover nanoparticles anchored on MoS2 layers for heterostructures with tunable strain driven by thermal or light induced spin switching

Strain engineering has become a powerful strategy for the controlled modification of the lattice structure and, consequently, of the optoelectronic properties of 2D materials. Different setups have been reported to induce mechanical strain on the layers. However, so far, a synthetic approach to prepare self-strainable 2D layers had not been faced. In this work, we have relied on the chemical functionalization to generate reversible strain on MoS_2. Therefore, semiconducting MoS_2 layers have been decorated with spin-crossover nanoparticles (SCO-NPs) to exploit the ability of spin-crossover molecules to switch between two spin states upon the application of external stimuli, giving rise to a smart hybrid self-strainable 2D system (Figure 2).

In the resulting hybrid material, the application of light or temperature leads to spin transition of SCO-NPs, which is accompanied by their volume change. This variation induces a modulation of strain over the MoS_2 layer, producing a dramatic and reversible modification of its electrical and optical properties. These changes can be followed by means of transport and photoluminescence measurements. SCO-NPs of different sizes combining different degrees of MoS_2 surface coverage have been studied to evaluate the influence of the molecular counterpart. This novel class of smart hybrid 2D composite could open the way to the synthesis of a broad number of hybrid multifunctional self-strainable 2D materials with potential application in different technological fields like sensing, optoelectronics or spintronics (see line 4). [11]

This hybrid SCO/2D approach has been exploited to prepare robust electronic nanodevices based on SCO in Line 4.

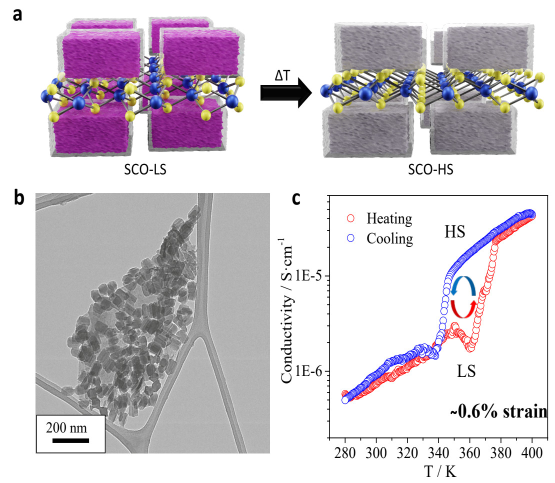

Figure 2. (a) Illustration of the hybrid SCO/MoS_2 heterostructure showing the termal spin transition; (b) Real transmission electron microscopy image of the heterostructure. (c) Thermal-dependent electrical conductivity of the SCO/MoS_2 hybrid showing the electrical detection of the spin transition.

3. Outlook

This line has been mainly developed by four groups (Navarro-Moratalla, Abellán, Baldoví and Coronado) within the frames of their ERC projects. Groundbreaking results have been obtained dealing with the physics of 2D magnets (including 2D MOFs), the chemistry of 2D materials (in particular, 2D pnictogens), the design of a novel class of molecular/2D heterostructures that respond to physical stimuli, and the development of efficient electrocatalysts based on Layered Double Hydroxides (LDHs) for water splitting. This last application has been at the origin of the spin-off company 2D-MATCH, which has evolved recently to MATTECO. Finally, since this line is strongly focused on magnetic materials, it is closely connected with line 4 (Molecular Spintronic Devices).

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LINE 3. MOLECULAR DESIGN OF BIOMATERIALS

1) Introduction

Since the foundation of the ICMol, this line has been fundamentally based on supramolecular chemistry and the design of metal complexes for biomedical application. Our staff now provides the additional expertise required to tackle an innovative research program that aims to develop advanced biomaterials for immediate impact on areas of strategical value as chiral separation, delivery of biologically active molecules, biomedicine, biocatalysis and/or biosensing. In other words, we intend to work at the interface between molecular chemistry, biology and materials science with specific focus in the following topics:

O3.1) Porous crystals based on peptide connectors for selective recognition of biomolecules: design of biomimetic porous frameworks capable of adapting their structure to environmental changes whilst maintaining long-range periodicity. Our previous works in MOF chemistry confirm the suitability of oligopeptides to confer controllable structural responses to guest uptake that can discriminate enantiomers to enable efficient separation of chiral drugs or activate small substrates for enantioselective catalysis.

O3.2) Stabilization and controlled release of biologically active macromolecules for biomedical applications: Joint efforts combining expertise in supramolecular and reticular chemistry will be used to design porous hosts, hydrogels and liposomal formulations for enhanced biocompatibility and more selective recognition of guests to gain control on their release kinetics. This goal will specifically encompass the use of drugs, antibiotics, antifungal, antimicrobial and inorganic biomimetic complexes with anticancer, antiparasitic/antitumoral activity or antioxidant activity for the treatment of neurological disorders. Host design will also involve the shaping and modification of their surface chemistry to tune their interaction with cells and tissues relevant to safety, biodistribution, and efficacy.

O3.3) Advanced biocatalysts (superenzymes) of relevance in food industry, synthesis of biofuels and nitrogen fixation: Enzymatic catalysis is of great importance to the chemical industry, but broader application remains restricted by the poor stability of enzymes for poor cyclability and narrow operational range. Immobilization of enzymes in porous hosts or the generation of biomimetic catalytic sites in their structure can lead to efficient stabilization, prevent undesirable leaching, self-aggregation and enhance substrate selectivity due to size restriction. By using this strategy and biomimetic mineralization, advanced enzyme biocatalysts are intended to be developed from encapsulation of proteases (food industry), xylanases (biofuels) and nitrogenases (reduction of N_2 to NH_3).

O3.4) Optical control of biomolecules: use of light-sensitive proteins and peptides, photoswitchable lipids and photoacids to study the interaction, folding, functionality and/or transport in membranes. As light can be delivered with high spatial and temporal precision, the optical control of biomolecules will be used for the optical manipulation of biomaterials containing light-sensitive proteins and peptides and for the light-controlled uptake/release of guests.

2. Highlights

Biomimetic catalysis in titanium-organic frameworks

Heterometallic metal-organic frameworks (MOFs) can offer important advantages over their homometallic counterparts to enable targeted modification of their adsorption, structural response, electronic structure, or chemical reactivity. We have designed a new family of mesoporous titanium-organic frameworks, MUV-101(M), that displays heterometallic TiM_2 nodes assembled from direct reaction of Ti(IV) and M(II) salts. We use the degradation of nerve agent simulants to demonstrate that only $TiFe_2$ nodes are capable of catalytic degradation in non-buffered conditions.[1] This activity cannot be explained only by the association of two metals, but to their synergistic cooperation, to create a whole that is more efficient than the simple sum of its parts. Our simulations suggest a dual-metal mechanism reminiscent of bimetallic enzymes, where the combination of Ti(IV) Lewis acid and Fe(III)–OH Brönsted base sites leads to a lower energy barrier for more efficient degradation of DIFP in absence of a base.

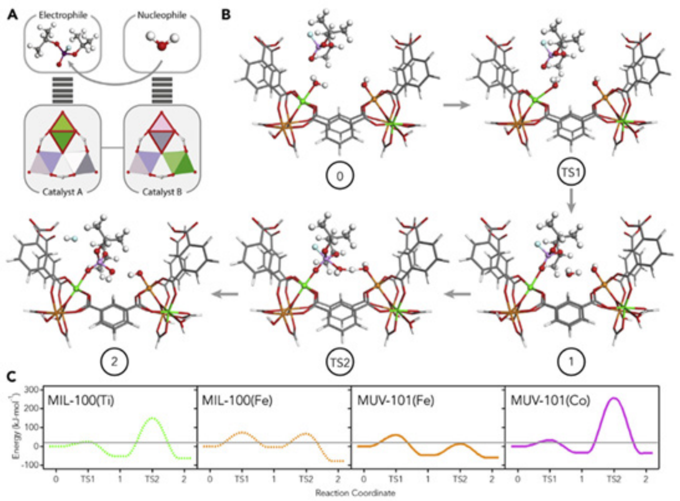

Figure 1. Proposed Mechanism for Dual-Metal Catalytic Detoxification in Heterometallic MUV101(Fe). a) Cooperative action of neighbouring metal sites. b) Proposed reaction mechanism for biomimetic dual-metal degradation of organophosphorus compounds. c) Reaction energy profiles for MIL-100(Ti) and heterometallic MUV-101(M) analogues.

Growing and shaping peptide MOFs at the millimeter scale

We show that environments mimicking microgravity conditions can harness the size and shape of functional biogenic crystals such as peptide-based metal-organic frameworks (MOFs).[2] We demonstrate formation of the largest single crystals with controlled nonequilibrium shapes of peptide-based MOFs reported to date, as opposed to the typical polyhedral microcrystals obtained under bulk crystallization conditions. Our method mimics two main strategies of morphogenesis in biomineralization, i.e., spatial, and morphological control, both being largely unexplored in the field of self-assembled functional materials. These results offer new opportunities to study and understand fundamental questions of how the size and shape of artificial crystals can influence their properties while providing a strategy to tailor the size and shape of peptide-based MOF single crystals to specific applications as chiral stationary phases for chromatographic separations.

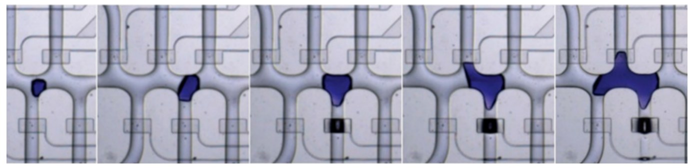

Figure 2. Controlled growth and shaping of Cu(Gly-L-HisGly) crystals in a microfluidic device.

Optical control of the location of a protein fragment in a lipidic membrane

The spontaneous insertion of helical transmembrane (TM) polypeptides into lipid bilayers is driven by three sequential equilibria: solution-to-membrane interface (MI) partition, unstructured-to-helical folding, and MI-to-TM helix insertion. A bottleneck for understanding these three steps is the lack of experimental approaches to perturb membrane-bound hydrophobic polypeptides out of equilibrium rapidly and reversibly. We have synthetized a 24-residues-long hydrophobic α-helical polypeptide covalently coupled to an azobenzene photoswitch (KCALP-azo). We have demonstrated spectroscopically that this polypeptide folds as a TM α-helix (TM topology) when the azobenzene is in trans conformation, but that after trans-to-cis photoisomerization with UV light it moves to the membrane interface, a process reversed with blue light.[3] We are using this new light-controllable system to address the molecular mechanism and kinetics for the membrane insertion of peptides into lipidic membranes.

Novel optical probes to tackle non-canonical DNA

Non-canonical DNA and RNA structures such as G-quadruplex play key roles in some biological processes such as telomere maintenance and oncogene expression. Nevertheless, the lack of tools to visualize them in cells hampers to gain a better knowledge of their potential applications as therapeutics. We have developed several probes based on triphenylamine[4] and triangulenium[5] scaffolds to detect, quantify and visualize G-quadruplexes in live cells. The results highlight the importance to develop molecules with a strong binding to G4s and selectivity over other biomolecules to afford good G4 probes as well as the relationship between G4 folding and *FancJ* and *RTEL1* helicases, which are directly associated to genome stability and cancer.

Advanced drug delivery systems for treating diseases

We have developed amino-nanozyme systems to eliminate unbalanced reactive oxygen species and treat neurodegenerative disorders. Macrocyclic metal complexes supported in boehmite nanoparticles show ability to remove MitoROS and to disaggregate inclusion bodies generated in Huntington disease.[6] In addition, we developed new upconversion nanoparticles coated with cucurbituril for biological applications.[7] We assessed the biological activity and concluded that they can be applied to bioimaging platforms for two-photon fluorescence microscopy.

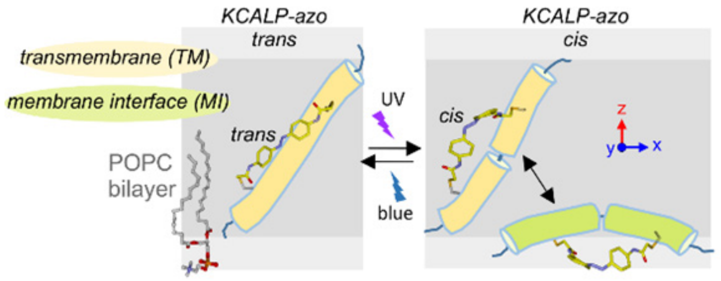

Figure 3. Structural models of the photoswitchable peptide KCALP-azo in trans-azobenzene and cis-azobenzene states in a lipid bilayer

Hierarchical mesoporous MOF for the selective delivery of macromolecular drugs

MOFs have received attention as drug delivery systems, as these porous crystalline hybrid solids can store high drug payloads. Despite the interest raised, their application in the delivery of macromolecules is limited by their pore size and opening. Herein, we present the synthesis of nanostructured MUV-2 [8], a hierarchical mesoporous iron-based MOF that can store high payloads of the macromolecular drug paclitaxel (ca. 23% w/w), increasing its selectivity towards HeLa cancer cells over HEK non-cancerous cells. Moreover, this NanoMUV-2 permits full degradation under simulated physiological conditions while maintaining biocompatibility, and is amenable to specific surface modifications that increase its cell permeation, efficient cytosol delivery and cancer-targeting effect, further intensifying the cancer selectivity of paclitaxel and opening the door for PTX resistance studies.

Biomineralization of MOFs for the hierarchical organization and protection of biomolecules

Nature has selected biomineralization as an extremely effective tool to hierarchically organize biomolecules, enabling biological function. Although limited to specif architectures, this concept has been developed to MOFs for the preservation and controlled release of specific bioentities.[9,10] We have developed a general Lewis-acid mediated in situ strategy that promotes the spontaneous growth of a broader number of MOF structures on previously inaccessible proteins. We demonstrate the ability of the MOF scaffold to retain bioactivity while enableing biomolecule controlled delivery for therapeutic or catalytic use.

Suistained release of antimicrobial agents for food packaging

The design of efficient food contact materials that maintain optimal levels of food safety is of paramount relevance to reduce the increasing number of foodborne illnesses. We have develop a MOF-based composite that fosters a unique prolonged antibacterial activity against Escherichia coli and Listeria innocua. This is possible due to the intrinsic redox nature of MIL-100(Fe), that triggers a two-step carvacrol release from films containing the carvacrol@MOF composite. The combination of a direct preparation, facile processing, and the MOF-mediated prolonged carvacrol bactericidal activity makes the composite a promising candidate for food packaging applications. [11]

ERC Consolidator Grant to LIVINGPORE

The project aims to develop innovative strategies to “program” the chemistry and the structural response of Metal-Organic Frameworks. The central objective of this materials chemistry project is to lay definitive understanding on how reticular frameworks can be used to respond to or select specific molecular recognition patterns for cooperative selection in a crystalline solid. The long-term vision is a shift in the present perception of MOFs into unique porous materials capable of structural/functional responses closer to biological systems that enable distinctive applications currently unthinkable of, that will be initially demonstrated in separation and biocatalysis.

Biotechnology for cleaning and disinfection of pathogens

This cooperative strategic project joints efforts from different companies, public research organisms, technological institutes and University. The project aims to develop integral biotechnological systems based on the effective use of endolysins against resistant pathogens in food and clinical sectors. ICMol leads the design and development of bio-composites based on porous materials for the preservation and controlled delivery of the endolysins, ensuring their practical use in disinfectant products. The final goal is to provide solutions to ensure the safety of food products and in clinical practices and environments.

LIVINGPORE

Figure 4. Logo of the ERC project LIVINGPORE.

PMA start-up to accelerate technology transfer

On November 2021, the University of Valencia (UV) established and recognized as a spin-off the chemical company Porous Material in Action (PMA). Mainly participated by researchers from the ICMol and by the University itself, the company aims to produce MOF-type porous materials, place value on them for their integration into technological applications and make them affordable to the industry. In addition to assuming the challenge of producing them at an affordable cost, PMA (www.porousin-action.com) is committed to making these highly versatile and highly capable materials known to the industry in general. This initiative has been the winning project of the 7th VLC-Startup award organized by the Parc Científic of University of Valencia and Banco Santander.

Figure 5. Birth of Porous Materials in Action, first Spanish initiative dedicated to MOF valorization.

Research Lines

New porous platforms for active encapsulation of enzymes

One of the main limitations of the integration of enzymes or macromolecules into porous materials is the size limitation of the pore volumes accessible in molecular frameworks. We have developed new titanium MOFs that grant access to mesoporous cavities with internal diameters close to 3 nm and good chemical stability in aqueous solutions. [12] In parallel, we also developed an alternative post-synthetic modification methodology that enables the use of tetrazine groups as reactive tags for the diversification of pore chemistry by click reactions with a broad scope of functionalities. [13]

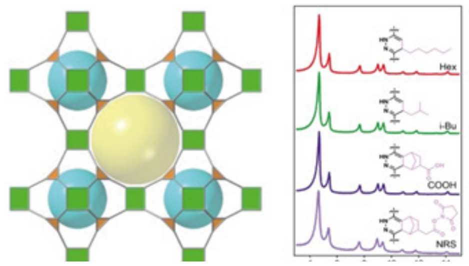

Figure 6. Topology of ultraporous titanium frameworks and new tetrazine post-synthetic ligation chemistry adapted to pore diversification

3. Outlook

Besides early scientific achievements accomplished in these first 2 years, the creation of a start-up to facilitate the transfer of results to non-academic partners, and the award of different projects that encompass some of the targets propose constitute a solid platform to accelerate the development of this research line soon. There are three main directions that will be developed further. We are confident the design of porous, flexible biomimetic materials with programmable pore chemistry (1) might lead to high selectivity in the recognition of guests not only controlled by size but also by chemical interactions that respond to fit-induced response of the framework. This exquisite control might lead to unprecedented opportunities in separation and biocatalysis. Our results in the optical control of the conformation of proteins will be used to extend this behavior to short chain synthetic polypeptides. They will be used as connectors in molecular frameworks to combine structural flexibility with optical response to access light control over guest recognition (2). Finally, we expect our ongoing work with molecular frameworks and complexes for the treatment of diseases and encapsulation of biologically active molecules to benefit from these new strategies to gain chemical control over guest uptake/release for targeted dosing (3). Previous and newly defined goals will all benefit from the incorporation of a computational chemist with expertise in Molecular Dynamics that has been integrated in the research line by early 2023 (Dr. Misturini). Also, the recent award of an ERC CONS will be used to purchase new equipment to fill the gaps identified during the first stage of the MdM project.

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LINE 4. MOLECULAR SPINTRONIC DEVICES

1. Introduction

Molecular spin-based electronics merges conventional spintronics with molecular magnetism and molecular electronics. This line intends to evolve from the study of the fundamental processes involved in the spin injection and transport through molecules (targets of the spintronics line in our previous MdM project), to the fabrication of novel classes of molecular spin devices.

Specific research objectives and priorities of Line 4 are:

O4.1) Fabrication of multifunctional spintronic devices. The advances in the fabrication of molecular analogues to the inorganic spin valves have benefited from the advances performed in the design and study of the hybrid organic/inorganic interfaces. A strong effort has been performed to tailor and optimize the spin transfer at the hybrid interface. The next step that we propose here is to develop new smart interfaces based on multifunctional molecular materials, in particular stimuli-responsive magnetic materials, to fabricate multifunctional spin valves that can be addressed through external stimuli. Thus, we will explore the insertion of ultra-thin films of spin-crossover molecules in between the two ferromagnetic electrodes. This study comprises the design of the appropriate molecules that are compatible with the high vacuum techniques required in spintronics, the processing of the materials over surfaces and, finally, the characterization of the devices.

O4.2) Fabrication of nanoscale spintronic devices based on coordination chemistry. We propose to integrate functional molecules into nanospintronic devices. In particular, we will focus on the chemical design and functionalization of the magnetic molecules in order to make them suitable for their integration in tunneling devices. A second objective will be that of integrating also the 2D magnetic materials prepared in Line 2, in particular those based on coordination chemistry.

2. Highlights

Design of spin-crossover systems for their deposition over surfaces as ultra-thin films

A promising approach to spintronic devices is addressed to the development of new smart interfaces with stimuli-responsive magnetic properties based on spin crossover (SCO) systems.

The SCO transition represents one of the most spectacular examples of molecular bistability in response to external stimuli (T, P, irradiation with light, electric fields, guests-molecules, etc.) where, in the case of some Fe(II) compounds in an octahedral environment, there is a transition from a paramagnetic high-spin (HS) state with an open-shell configuration—$(t_{2g})^4(e_g)^2$—to a diamagnetic low-spin (LS) one with a closed-shell configuration —$(t_{2g})^6$— (Figure 1top).

Hence, the synthesis of stable SCO molecules that permit their integration as ultra-thin films in between ferromagnetic electrodes keeping their switchable properties is a key goal in the fabrication of new types of spin valves.

Here we have explored the growth of 2D Hofmann-Type iron (II) SCO Materials using solution methods. Two new series of cooperative SCO 2D Fe^{II} coordination polymers formulated as $\{Fe^{II}(Pym)_2[M^{II}(CN)_4]\cdot xH_2O\}_n$ and $\{Fe^{II}(Isoq)_2[M^{II}(CN)_4]\}_n$ (Pym = pyrimidine, Isoq = isoquinoline; M^{II}= Pd, Pt) have been synthesized [1]. The corresponding Pt derivatives have been selected for fabrication of thin films by liquid-phase epitaxy. At ambient pressure, the microcrystalline materials of both series display strong cooperative thermal induced SCO properties. The SCO behavior of the thin films is maintained but with the spin transition appearing at lower temperatures than the corresponding microcrystalline samples. Furthermore, whereas the previously reported $\{Fe^{II}(Py)_2[Pt^{II}(CN)_4]\}_n$ (Py = pyridine) films retain interesting cooperative and reasonably complete SCO properties, a noticeable increase of inactive HS Fe^{II} centers is observed for the Pym-Pt and Isoq-Pt derivatives inducing a complete loss of cooperativity for the latter despite the great structural resemblance of the three compounds. These findings represent a cautionary tale for further work with films of other SCO systems grown via Layer-by-Layer method (LbL).

We have also designed a sublimable molecule that forms very homogeneous ultrathin-films using high-vacuum technique [2]. The neutral Fe(II) complex can be formulated as $[Fe(neoim)_2]$, where neoimH is the ionogenic ligand 2-(1H-imidazol-2-yl)-9-methyl-1,10-phenanthroline. This complex forms thin films through high-vacuum sublimation that retain the SCO capabilities of the bulk. In particular, a very efficient and fast light-induced spin transition (LIESST effect) has been observed, even for ultrathin films of 15 nm. We are currently exploring the possibility of using this molecule to fabricate spin valve devices responding to light.

Chiral paramagnetic metallopeptides for room-temperature spintronic devices.

In last years the spintronics community has payed attention to the potential of chiral molecules to polarize the spin of electrical current, the so-called Chirality-induced spin selectivity effect (CISS). We have explored the use of self-assembled monolayers (SAMs) of helical lanthanide-binding peptides (LBT) to study the influence of metallic dia- and paramagnetic centers as additional parameters on the control of the spin transport.

First, a cysteine terminal amino acid has been added in the LBT sequence to work as anchoring point on gold protected nickel surfaces, driving the self-assembling process. We have prepared SAMs of LBT coordinating diamagnetic Y^{3+} and paramagnetic Tb^{3+} ions, which have been deeply studied by several surface characterization techniques (atomic force microscopy, X-ray absorption spectroscopy, quartz crystal microbalance measurements…). CISS effect has been proved by means of spin dependent electrochemistry: cyclic voltammetry and electrochemical impedance measurements. Additionally, we have implemented the standard liquid-metal drop electron transport setup, demonstrating the possibility of spin-dependent local transport in solid-state devices. These independent techniques suggest that the spin polarization in enhanced when a paramagnetic center is included in the peptide. These results incorporate magnetic biomolecules in the CISS field and pave the way to their implementation in a new generation of (bio) spintronic devices [3].

Hybrid molecular/2D heterostructures: when spin-crossover molecular systems interact with 2D materials

Conventional van der Waals heterostructures combine deterministically different inorganic 2D materials with the aim of exploring the new emerging physical properties that can appear due to proximity effects, as paradigmatically exemplified in magic angle twisted bilayer graphene. In this scenario, molecular magnetic compounds can be added as novel building blocks bringing new physical properties, as the so-called spin-crossover phenomenon (see previous description). This crossover leads to a compression/expansion of the metal site and, consequently, of the crystal lattice upon the spin transition.

Thus, SCO materials can be envisaged as molecular building blocks able to produce strain to other 2D materials. We have demonstrated it by placing deterministically a SCO thin-layer of the 2D Hofmann-Type metal-organic framework $\{Fe\text{-}(3\text{-}Clpyridine)_2\text{-}[Pt^{II}(CN)_4]\}$ together with few-layers graphene or monolayer WSe_2. By tracking the electronic properties in former and the photoluminescence in the latter, the properties of the 2D inorganic materials are clearly switched when the spin transition takes place. This is attributed to the strain generated by the molecular layers due to the volume change concomitant with the spin transition. In the case of few-layers graphene, this strain shifts the Fermi level, while in WSe_2 monolayers it changes the band structure (Figure 1bottom) [4].

However, despite the above-mentioned result, the fragility of SCO compounds upon thermal treatment, light irradiation or deposition on surfaces and the techniques used for their processing have limited their applicability. To overcome these limitations we have fabricated hybrid devices with outstanding performance based on the sublimable and robust SCO $[Fe(Pyrz)_2]$ (Pyrz = hydro-tris-(3,5-dimethyl-pyrazolyl)borate) molecule deposited over CVD-graphene. In this way, it is possible to downsize the thickness of these hybrid heterostructures below 100 nm. Moreover, this novel methodology allows us to electrically detect a fast and effective light-induced spin transition in these devices (~50 % yield in 5 minutes). Such performance can be improved reaching an unprecedented yield of ~100 % in 5 minutes using a contactless configuration, by inserting a flexible polymeric layer between the two active components, which should facilitate the volume change of the SCO film in the spin transition [5]. This novel approach has been outlined in [6].

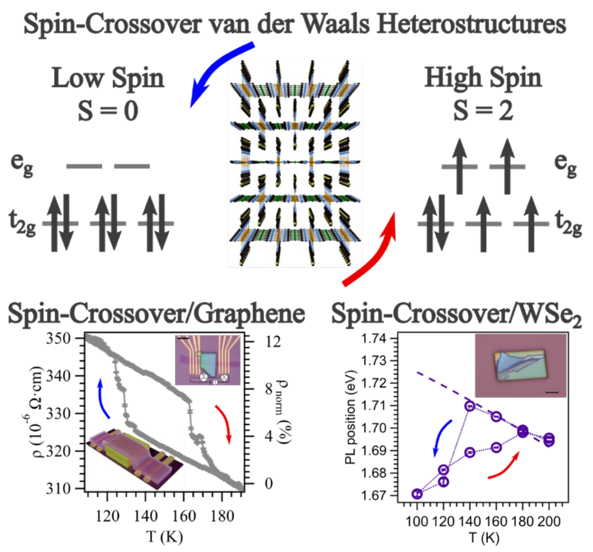

Figure 1. Spin-crossover van der Waals heterostructures. Top: Scheme of the spin crossover transition together with the crystal structure of the spin-crossover metal organic framework {Fe-(3-Clpyridine)$_2$-[Pt^{II}(CN)$_4$]}. Bottom: hybrid molecular/inorganic van der Waals heterostructures where the spin transition can be detected by electrical transport (graphene case) and optical measurements (monolayer WSe$_2$ case).

Overall, SCO layers are a new building block able to induce strain in 2D heterostructures, thus paving a new avenue in the emergent fields of straintronics and band engineering in low-dimensional materials. This gives rise to the fabrication of hybrid devices which allow a highly sensitive platform both to detect the spin transition of the molecular component (SCO), and to tune the properties of the 2D material and open the possibility to obtain novel smart hybrid interfaces in spintronic devices.

Van der Waals spin valves: Controlling the properties by twisting 2D magnetic layers

As pointed out in Line 2, 2D magnets is a hot area of research in the field of 2D materials. We have recently showed that bilayers of the semiconducting coordination compound CrSBr, integrated into electronic nano-devices, exhibit a spin valve behaviour (Figure 2). Each single layer is ferromagnetic up to T_C ~150 K and has uniaxial anisotropy with the spins pointing along the easy b axis, whereas the two layers couple between them antiferromagnetically. By applying a magnetic field, it is possible to flip the layers' magnetization in a parallel fashion via a spin reversal along the magnetic field direction. This spin flip is accompanied by a sharp decrease of ca. 40% in the magnetoresistance at 0.2 T when the field is applied along the easy b axis and does not present hysteresis (Fig. 2, right) [7].

A groundbreaking result has been obtained by twisting 90 degrees two CrSBr ferromagnetic monolayers. As a result, the easy axis of the two layers is rotated 90 degrees. This leads to emergent properties sharply different from those shown by the pristine case. In fact, the magneto-transport properties reveal multistep magnetization switching with a magnetic hysteresis opening, that is absent in the pristine case, together with a linear dependence of the resistance vs field (at low fields), providing thereby a magnetic field sensor (Figure 2, center). These results highlight the potential of using twist angles as a key design parameter for van der Waals spin valves and open the field of spin twistronics [8].

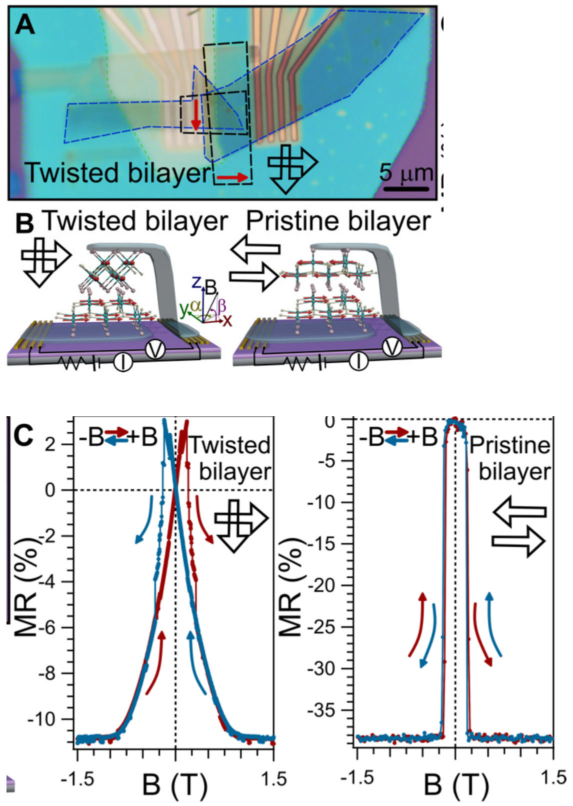

Figure 2. Magnetic switching control by twisting CrSBr layers. (A) Optical image: example of a 90° twisted bilayer device; (B) Sketch of a 90°/0° twisted/pristine bilayer (left/right); (C) Magneto-resistance measurements for a twisted/pristine (left/right) bilayer for fields along α = 90° β = 0° (as sketched in b) and T = 10 K. adapted from refs. 7 and 8.

3. Outlook

The research in molecular spintronics have resulted in significant advances both from the point of view of the materials as well as from the point of view of the devices. Thus, novel spin-crossover materials have been designed exhibiting unique chemical properties (as for example, robust sublimable molecular complexes showing very efficient photomagnetic effects, as well as strong thermal stabilities; or layered MOFs that can be exfoliated to form van der Waals heterostructures when combined with graphene and other 2D materials), or chiral metal-coordinated biomolecules showing CISS effect. On the other hand, spin devices based on SCO/2D heterostructures have been prepared. This approach has shown to be very suitable to obtain for the first time, resilient nano-scale SCO electronic devices in which the spin state can be electrically detected without compromising the stability of the SCO complex. Finally, we have pioneered the design of twisted spin valve devices based on 2D ferromagnetic inorganic complexes by twisting two vdW layers by 90º. This spin-twistronics engineering provides a versatile approach to tune the magnetoresistance properties of this new type of spin devices.

This work has been mainly developed in the frame of the ERC advanced grant MOL-2D (to Coronado) and the European FET-OPEN Projects COSMICS and SINFONIA (led at the ICMol by Coronado, in collaboration with the coordination chemistry group led by J. A. Real, and with the theoretical support of J. J. Baldoví, ERC starting grant SMARTIES).

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Research Lines

LINE 5. MOLECULAR SPINS FOR QUANTUM TECHNOLOGIES

1. Introduction

Spins provide one of the simplest platforms to encode a quantum bit (qubit), the elementary unit of second generation quantum technologies, including quantum computers. Still, performing any useful quantum operation demands much more than realizing a robust qubit. Quantum logical operations or "qugates" between two qubits are also required, and eventually one will need a large number of qubits and a reliable procedure to integrate them into a complex circuitry that can store and process information and implement quantum algorithms. This scalability is arguably one of the challenges for which a chemistry-based approach is best-suited. Molecules, being much more versatile than atoms, are the quantum objects with the highest capacity to form non-trivial ordered states at the nanoscale and to be replicated in large numbers. Over the last decades, Molecular Magnetism has produced an array of tools to design and fine-tune magnetic molecules, in particular, molecular nanomagnets. Indeed, the design of robust molecular spin qubits is a natural evolution of the molecular engineering of nanomagnets.

Specific research objectives and priorities of this research line included:

O5.1) Identification of key chemical design strategies for engineering slow spin relaxation and long coherence times at a molecular scale. For reaching this goal we will build upon our already existing pioneering breakthroughs on modelling the coupling between spin states and molecular distortions, including molecular vibrations.

O5.2) Design of robust molecular spin qubits showing long coherence times. To reach this goal a five-step process is required: i) the chemical design of crystals containing the magnetic molecules of choice (lanthanoid polyoxometalates (POMs) and endohedral metallofullerenes); ii) the magnetic characterization of these systems using both magnetic and spectroscopic techniques, iii) the qubit manipulation using pulsed EPR, iv) the integration of the molecular system in a superconducting resonator setup; v) the theoretical modelling of the time evolution of quantum spin states.

O5.3) Design of multi-qubit molecules. Molecules with large spin Hilbert spaces, often through a combination of electronic and nuclear spins, provide a unique opportunity to get multiple addressable quantum states in a single molecule. This unique feature, allows to implement quantum operations within a single molecule as it behaves as a multi-qubit processor. In order to design multi-qubit molecules, the chemical, structural and electronic requirements need to be established. Then, their spin states should be addressed using pulsed EPR.

2. Highlights

Design, preparation and characterization of qubits based on POMs

Molecular spin qubits that can be controlled electrically are typically susceptible to decoherence, since electrical noise is more pervasive than magnetic noise. We found that certain holmium molecular spins provide a solution to this apparently fundamental contradiction by combining robust coherence with strong spin–electric coupling. Moreover, we do not rely solely on electric fields for manipulation, but rather employ a combination of microwave pulses and electric field pulses. Our main contributions in this period have been based on the POM known as HoW_{10}. This is a molecular nanomagnet in which a small structural distortion establishes so called "clock transitions" (that is, transitions whose energy is to first order independent of the magnetic field) in the spin spectrum. The fact that this distortion is associated with an electric dipole allows us to control the clock-transition energy to an unprecedented degree via an external electric field. By means of a collaboration with the team of A. Ardavan, Oxford Univ., we experimentally demonstrated coherent electrical control of the quantum spin state and exploited it to independently manipulate the two magnetically identical but inversion-related molecules in the unit cell of the crystal, see Figure 5.1 (pursuing O5.2). Our findings pave the way for the use of molecular spins in quantum technologies and spintronics. In view of these results we proposed the design of electrical two-qubit gates using a pair of clock-qubit magnetic HoW_{10} molecules within a diluted crystal (pursuing O5.3). ***The experimental result has been published in Nature Phys.*** [1] ***and the theoretical proposal in npj quantum information*** [2].

In another vein, we have been strongly involved in studying the interplay between spin states and vibrations (both phonons and molecular vibrations) since that constitutes an important source of decoherence. From a theoretical point of view, we have developed inexpensive first-principles method devoted to evaluating vibration-induced spin relaxation in molecular f-block single-ion magnets, with the important advantage of requiring only one CASSCF calculation [3], and in parallel worked on the design of further molecules presenting clock transitions [4]. Experimentally, we have identified the vibronic decoherence pathways and their coupling with the spin states in crystals of HoW_{10} by performing magneto-infrared measurements in collaboration with J. Musfeldt, Univ. Tennessee [5].

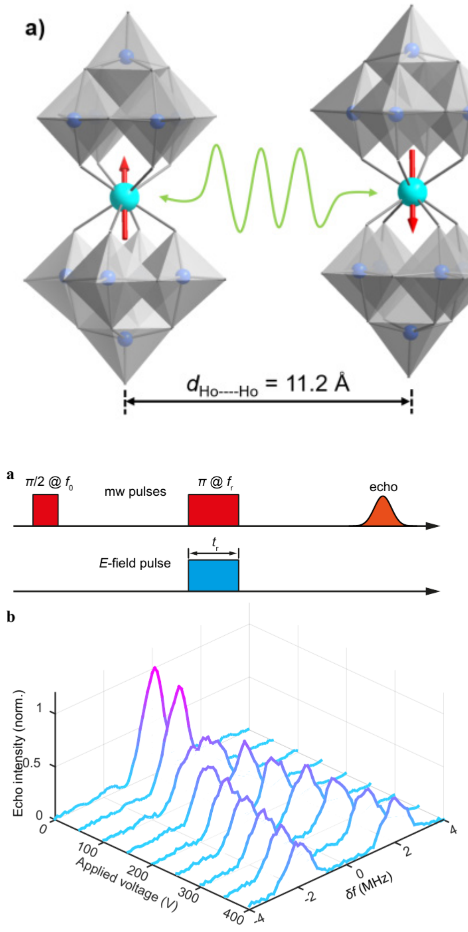


Figure 1.

(Top) Inversion-related pair of HoW_{10} POMs.

(Center) The modified Hahn-echo pulse sequence used for selective spin excitation in HoW_{10}. A p/2 pulse is applied at the CT frequency f0 , while the frequency of the refocusing p pulse, f_r , is swept. An E-field square pulse is applied simultaneously with the refocusing pulse to modulate the excitation frequencies of molecular spins. When $f_r = f_0 \pm df$, the refocusing pulse selectively inverts one or other of the inversion-symmetry-related molecular spins in the unit cell. (Bottom) The intensity of the spin echo as a function of the applied voltage, V , and the frequency offset of the refocusing pulse, df = $|f_0 - f_r|$. From ref. [1].

Qubits based on endohedral metallofullerenes

Endohedral metallofullerenes offer an excellent platform for molecular spin qubits thanks to the protection of nuclear spin-free carbon cage. Engineering their molecular structures via coordination chemistry is feasible to understand the underlying structural factors that govern the spin relaxation. To this end, a series of Eu(II)-based endohedral metallofullerenes $Eu@C_{2n}$ (2n = 74-90) have been synthesized. These complexes with slight anisotropy of the S = 7/2 spin have been characterized by EPR spectroscopy to show for the first time that Eu(II)-based complexes are alternative spin qubit candidates. More importantly, the rigidity of the three low energy metal-based vibrations are found to be controlled by the metal-cage binding structures, which play a crucial role in determining spin relaxation properties. Ab initio calculations at CASSCF level predict that $Eu@C_{74}$ (3) has a weaker spin-vibration coupling than $Eu@C_{84}$ (1) and $Eu@C_{82}$ (2). As a result, T_1 values for 3 are larger than for 1 and 2 in CS_2 solution. A universal behaviour for T_1 of these three complexes is obtained if temperature is normalized by frequencies of the three metal-based vibrations [6].

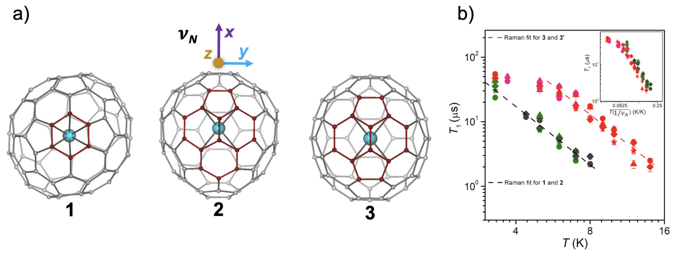


Figure 2. a) Molecular structures of $Eu@C_{84}$ (**1**), $Eu@C_{82}$ (**2**) and Eu@C74 (**3**) with three representative metal-cage binding sites highlighted in red. The three low energy vibrations in each molecule present metal movements along x-, y- and z-directions. b) Temperature dependence of T_1 of $Eu@C_{2n}$ molecules in CS_2 solution. The inset figure in d) shows the frequency-normalized T_1-temperature dependence, which is achieved through multiplying temperature by the averaged reciprocal frequencies of the three low energy metal-based vibrational modes.

Rational design, preparation and characterization of single-ion magnets

Higher T_1 values have been achieved by entrapping a single dysprosium (III) ion within a nitrogen-substituted carbon cage [6]. In this structure of $Dy@C_{81}N$, Dy^{III} is asymmetrically coordinated by one side to a hexagonal carbon ring of the azafullerene, while lacking any coordination ligand on the other side (Fig. 5.3). Due to this very unusual low-coordination environment, this compound exhibits a high blocking temperature of 45 K, the record value for any endohedral metallofullerene, despite a very weak energy barrier for the spin reversal. This opens a novel strategy to enhance the performance of single-molecule magnets at higher temperatures. This extraordinary magnetic behavior has been attributed to the minimal number of vibrations that couple to its spin states, which is also responsible for the unusual slow Raman relaxation mechanism observed at high temperatures. ***The results were published in Chem.*** [7]

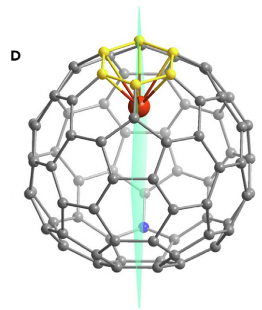
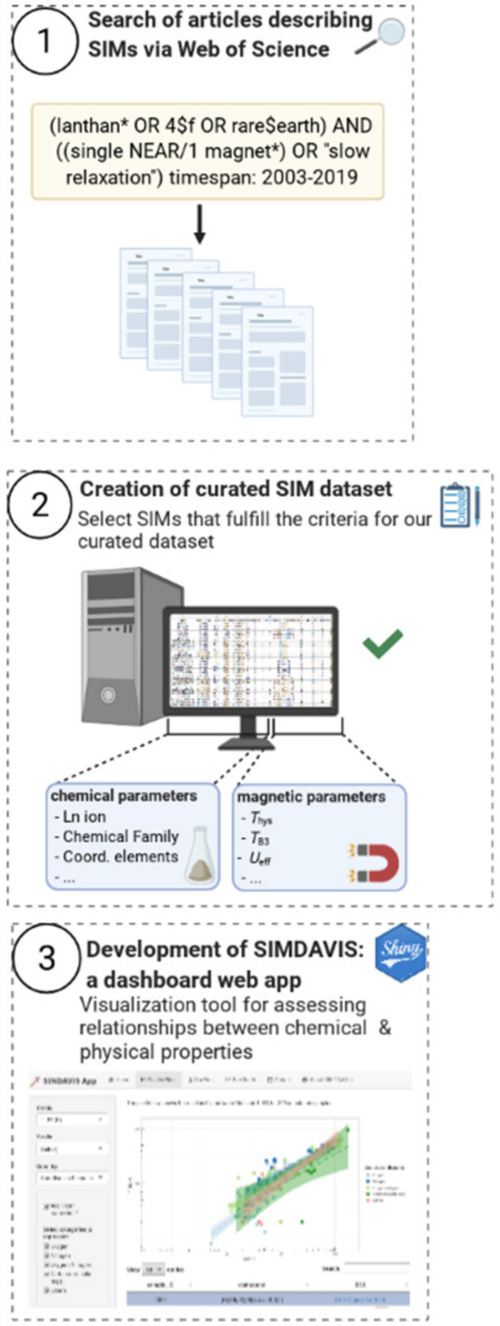


Figure 3. Structure of $Dy@C_{81}N$. Ref [7]

Data-driven design of molecular nanomagnets

Data science is revolutionizing our society, but the impact of cheminformatics is still limited mostly to drug discovery and bulk materials science, partly because of a scarcity in high-quality datasets. Over the last years, we have been preparing a contribution to what has been termed as the third generation computational chemistry: statistically driven design, applied to a hot topic within Coordination Chemistry, namely Single Ion Magnets. In order to establish a powerful framework for statistically driven chemical design of SIMs, we collected chemical and physical data for lanthanide-based nanomagnets to create a catalogue of over 1400 published experiments, developed an interactive dashboard (SIMDAVIS) to visualise the dataset, and applied inferential statistical analysis to it. The analysis opened up new questions, which we answered in a subsequent phase.



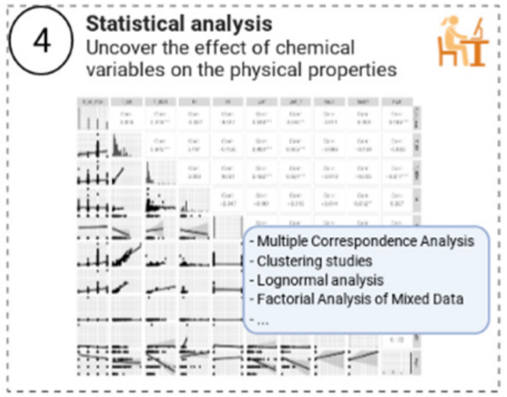


Figure 4. The 4 stages of our study, starting from the bibliography data mining, building the curated dataset, developing the dashboard web application with an user-friendly interface and finalising with the statistical analysis and the extraction of new insights.

From the study we were able to formulate a new hypothesis on the role of vibronic coupling, connecting the apparently independent roles of Orbach and Raman relaxation pathways. This study also offers several chemical design guidelines oriented towards the optimization of the effective barrier for the spin reversal in these molecules (U_{eff}) for the most common coordination numbers, in terms of chemical families and number of ligands. The results were published in Nature Communications [8].

3. Outlook

ICMol has been strongly involved in this topic through the ERC grant DECRESIM (2015-2021, to Gaita-Ariño) and also through two European projects (SUMO (2018-2021 and FET-OPEN FATMOLS, 2019-2023 coordinated at ICMol by Coronado) that intended to explore the possibility of using magnetic molecules to design robust spin qubits and scalable architectures to obtain a quantum spin processor. However, we failed to achieve either of the projected major milestones. Indeed, these goals have not seen the promised progress in these years. The molecular nanomagnet world record by the Layfield group mentioned in M5.1 dates from 2018 and has not yet been beaten by anyone worldwide. Similarly, the first implementation of a two-qubit quantum algorithm on a single molecule was achieved by the Wernsdorfer on 2017 and is still unsurpassed. Within this context we have been playing a role both in the chemical design of robust spin qubits, as well as in the theoretical modelling of their properties. In chemistry, we have profited from the unique electronic structure of a polyoxometalate featuring clock transitions and the possibility of electrically address the qubits in lanthanoid POM molecules, as well as magnetic nanomagnets based on endohedral metallofullerenes exhibiting relatively high-temperature magnetic blocking. From a theoretical point of view, we have made substantial advances on the important role played by the molecular vibrations in the spin relaxation processes and in the coupling between spin states, molecular distortions and electric fields, but there is still substantial room for improvement in the future.

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LINE 6. MOLECULAR ELECTRONIC DEVICES

1. Introduction

The specific research objectives and priorities of Line 6 are:

O6.1) Large area deposition of highly luminescent thin films. To enable the preparation of thin films of a wide range of semiconductors we will develop the processing tools, based on vapour phase deposition, implementing in-line real time monitoring using advanced spectroscopy tools such as hyperspectral imaging. The main objective is to achieve a process allowing for large area deposition of highly luminescent thin films (targets are PLQY >80%, areas $100 cm^2$, and thickness control <20 nm).

O6.2) Efficient and stable planar blue and white LEDs achieving a luminance >100000 cd/m^2, at >100 lm/W power efficiency and a stability in excess of 1000 hours. Current LEDs based on III-nitride semiconductors reach luminous efficiencies of 100-150 lm/W and are a mature technology. These LEDs are light-sources where the light originates from a central point. Alternative OLEDs using only organic semiconductors are planar emitters with efficiencies around 60 lm/W. Recently, red and green perovskite LEDs have been reported (also by us) with efficiencies in excess of 50 cd/A but with lifetimes below 1 hour. Hence, the main challenge is to extend the emission to the blue and to increase the stability. Here our objective is significantly beyond both technologies.

O6.3) Development of planar solar cells with efficiencies above >30% and a stability in excess of 1000 hours. Current PV devices are predominantly based on silicon with a record power conversion efficiency (PCE) slightly above 25%. To go beyond this level, devices employing different, complementary absorbers are needed in so-called tandem or triple junction devices. Perovskite semiconductors with the proper bandgaps can, according to calculations, raise the PCE of solar cells above 32%. For this, the cells must have a high luminous efficiency, as only then can the highest open circuit voltages (V_{oc}) be achieved.

O6.4) Demonstration of electrically pumped lasing in planar/thin film structures. This very challenging objective, would allow for the integration of lasers on flexible substrates generating a so far unexplored field of science and enable high volume applications.

2. Highlights

Large area Luminescent perovskite films

We have developed three new perovskite deposition methods that allow for large area thin films. Two are based on the mechanosynthesis of perovskite powders (a solvent free process) which are then converted into thin films by continuous flash evaporation,[1] or by hot pressing into thin disks.[2] A third method uses an in house developed close-space sublimation setup (the results obtained with this method were submitted in 2023 but only published in 2024 and therefore are not included in this report). Complementarily, the team of Julia Perez Prieto has developed perovskite nanoparticles absorbing UV light that emit in the blue range of the visible spectrum and can therefore be of potential interest for use as upconvertors in photovoltaic devices. A patent application has been applied for on this invention.

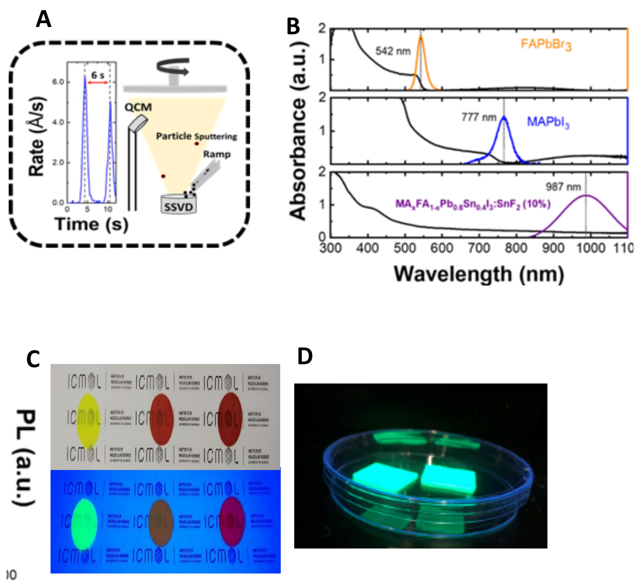

Fig. 6.1. A. Schematic of the flash feeder evaporation process and the deposition rate control, B: absorption and emission spectra of three perovskite composition prepared using the flash feeder and C: Photographs of the color converter disks based on perovskite polymer composites prepared using hot pressing, D. photograph of upconversion films employing perovskite nanoparticles.

Modelling of Charge transport in HTMs

We have developed a theoretical protocol to characterize and quantify the charge transport properties of hole-transporting materials (HTMs) as a function of temperature (dynamic disorder) and mesoscale morphology. In particular, the computational multiscale approach is based on molecular dynamics simulations, ab initio quantum chemical calculations of electronic coupling and reorganization energy, Marcus derivation of rate constants, and kinetic Monte Carlo simulations for hole mobility prediction. Our protocol was applied to archetypical spherical-like spiro-OMeTAD and a novel planar HTM based on the indoloindole core (IDIDF) (Figure 6.2). We demonstrate that the dynamic vibrations promoted by finite temperature leads to a decrease in the hole mobility up to one order of magnitude, as well as a significant increase in anisotropic transport, especially for spherical-like spiro-OMeTAD. On the other hand, fully amorphous phases further reduce the charge transport in around 3 orders of magnitude. Overall, IDIDF is predicted with two-orders-of-magnitude-enhanced hole mobility with respect to spiro-OMeTAD, in quantitative agreement with the experimental data, thus standing as a potential candidate for application in organic electronics and photovoltaics.[3] A preliminary protocol was applied to calculate the hole mobilities of hydrogen-bonded self-assembled HTMs that present robust semiconducting properties.[4]

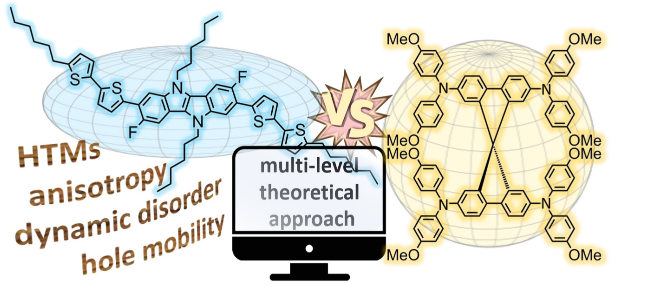

Figure 6.2. A multi-level theoretical protocol is developed to characterize the charge transport of hole-transporting materials as a function of molecular shape, dynamic disorder, and amorphousness. Chemical structures of IDIDF (left) and spiro-OMeTAD (right) are shown.

LEDs

In the area of LEDs, we have continued to collaborate with the group of Prof. Tae Woo Lee and have prepared perovskite based LEDs, exhibiting external quantum efficiencies in excess of 23% (and over 45 % with a hemispherical lens). High power efficiencies reaching > 90 lm/W are achieved and luminance levels up to 25000 cd/m2 with green light emitting perovskite nanocrystals, consisting of guanidinium inserted formamidinium lead bromide (Fig.6.2).[5]

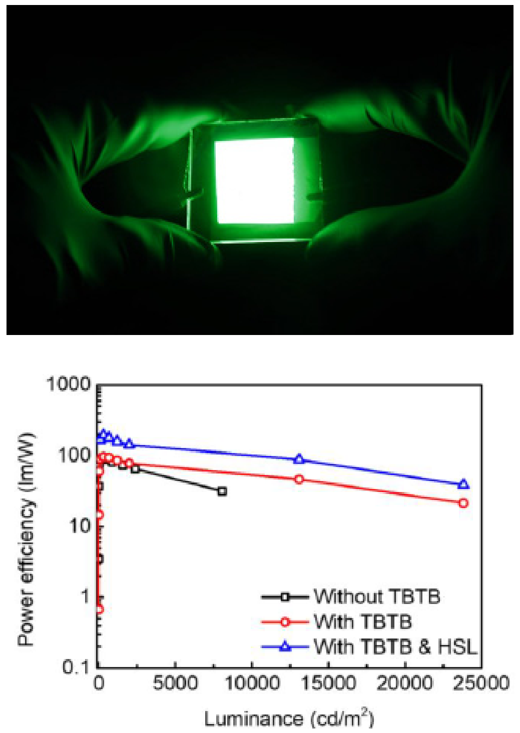

Figure 6.3. Top photograph of the perovskite based light emitting diode showing a record eqe at the time of publication. Bottom power efficiency as a function of luminance for this LEDs, both with and without 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (TBTB) and with a hemispherical lens (blue curve).

Photovoltaics

We have developed large area vacuum deposited perovskite solar cells, reaching power conversion efficiencies of 18 % for an active area of 21 cm² (Fig. 6.4A) This has been achieved using co-sublimation in a collaboration with the group of Prof. Mhaisalkar in NTU (Singapore).[6] Additionally, we have achieved efficient small area solar cells using multiple source sublimation methods.[7,8] An important achievement has been the development of a soft deposition method for transparent conductive oxides based on pulsed laser deposition.[9] This enable us to prepare LEDs and solar cells in which the top contact is semitransparent. We use this feature to prepare one of the first perovskite-perovskite tandems in substrate configuration. For this we have collaborated with the group of Prof. Wakamiya of Kyoto University who supplied us with the SnPb low bandgap perovskite bottom cells. After shipment from Japan to Valencia, we have deposited the charge recombination layer and the front wide bandgap perovskite cells using thermal sublimation and finished the device with the PLD deposited ITO layer (Figure 6.4 B, C and D).[10]

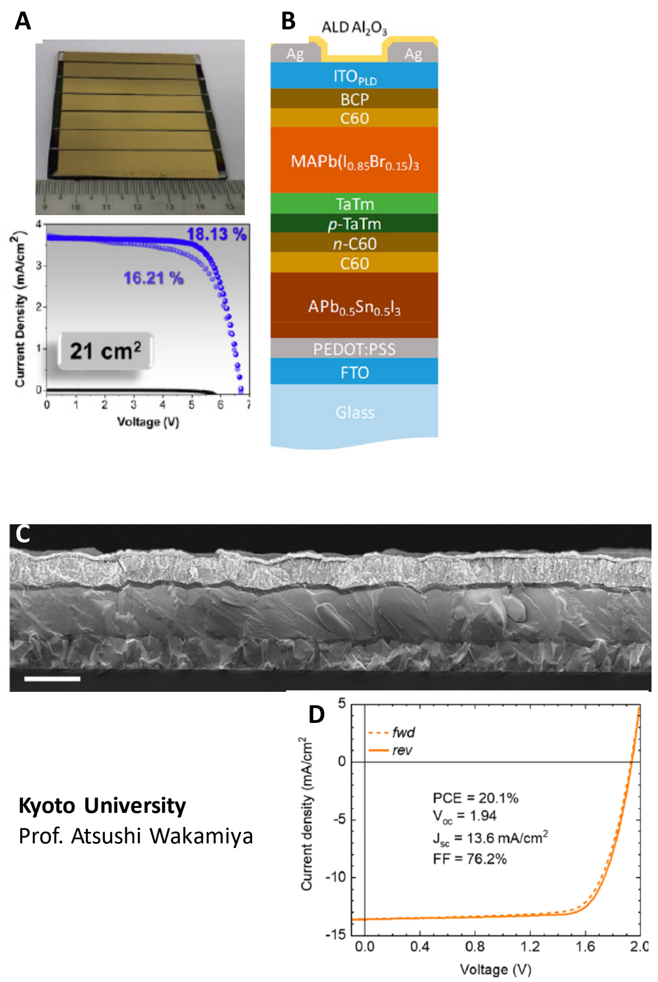

Fig. 6.4. A. Image of a minimodule of a perovskite single junction solar cell and J-V curve under 1 sun illumination, B: Layers used to prepare the perovskite-perovskite tandem cell C: SEM image of the cross section of the tandem cell, D. J-V curve of the tandem cell under 1 sun illumination and key performance parameters.

Lasing

The aim of electrically pumped lasing using perovskite based diodes has not been achieved; however, we did manage to prepare very interesting multilayer structures based on bi-layers of organic and perovskite semiconductors (Figure 6.5). In these stacks amplified spontaneous emission is observed using optical excitation. This work has been done in collaboration with the group of Dr. Annamaria Petrozza from IIT Milano.[11]

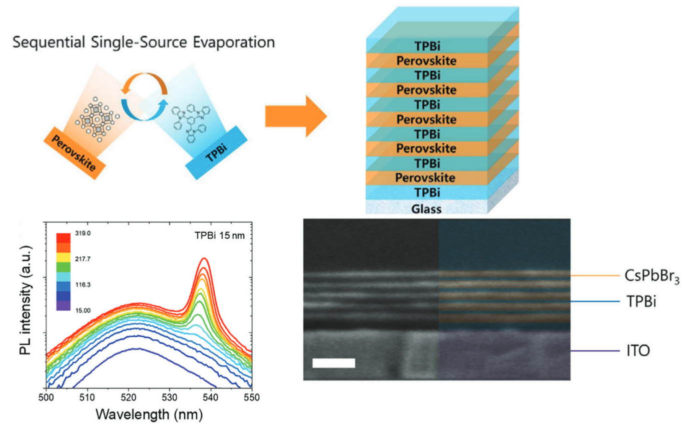

Fig. 6.5. Schematic of the co-sublimation process and the bilayer stack that was produced. Bottom, photoluminescence spectra at different excitation intensity showing the turn-on of ASE and a cross section SEM image of the bilayer stack.

3. Outlook

The research line "Molecular Electronic Devices" has involved the research groups of Prof. Enrique Orti, Prof. Julia Perez Prieto and Prof. Henk Bolink. Due to the interactions between these groups a better understanding of charge transport in molecular semiconductors and perovskites has been obtained. Progress in vacuum-based deposition methods for perovskite semiconductors and metal oxides has enabled the development of efficient photovoltaic devices. So far, however, the luminescence efficiency of vacuum deposited perovskite films is much lower than that of solution processed films containing nano-scale clusters/domains or particles. Due to this limitation, we have collaborated with expert groups working on solvent processed perovskite luminescent films to prepare efficient LEDs (Tae Woo Lee, SNU Korea). We are adopting the knowledge obtained in part thanks to the Maria de Maetzu project and through international collaborations, (Wakamiya, Kyoto, Petrozza, Milano, Mhaisalkar, Singapore) to our vacuum-based deposition processes to further enhance the luminescence properties of the perovskite films and enable their integration into thin film LEDs.

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5 reviews have been published related with this research line:

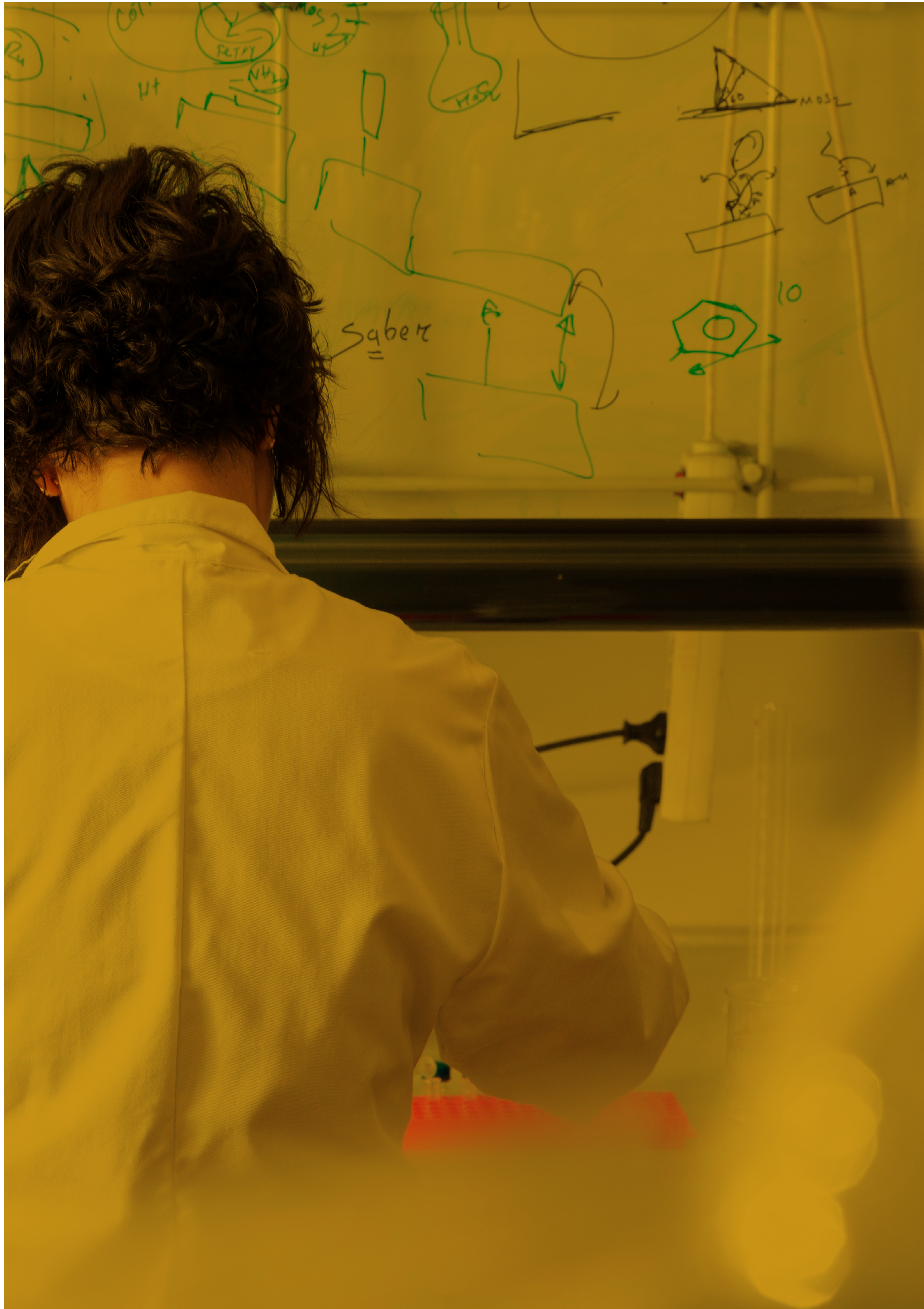
- *Applications of vacuum vapor deposition for perovskite solar cells: A progress review*. H. Li, M. Liu, M. Li, H. Park, N. Mathews, Y. Qi, X. Zhang, H. J. Bolink, K. Leo, M. Graetzel, Ch. Yi. ***IEnergy.*** *1 (4)*, 434-452 (2023).

- *Perovskite light-emitting diodes*. A. Fakharuddin, M. K. Gangishetty, M. Abdi-Jalebi, S.-H. Chin, A. R. bin Mohd Yusoff, D. N. Congreve, W. Tress, F. Deschler, M Vasilopoulou, H. J. Bolink. ***Nat. Electronics.*** *5 (4)*, 203-216 (2022).

- *Sputtered transparent electrodes for optoelectronic devices: Induced damage and mitigation strategies*. E. Aydin, C. Altinkaya, Y. Smirnov, M. A.Yaqin, K. P. S. Zanoni, A. Paliwal, Y. Firdaus, T. G. Allen, T. D. Anthopoulos, H. J. Bolink, M. Morales-Masis, S. De Wolf. ***Matter.*** *4 (11)*, 3549-3584 (2021).

- *Advances in solution-processed near-infrared light-emitting diodes.* M. Vasilopoulou, A. Fakharuddin, F. P. García de Arquer, D. G. Georgiadou, H. Kim, M. Yusoff, F. Gao, M. K. Nazeeruddin, H. J Bolink, E. H. Sargent. ***Nat Photonics***.*15 (9)*, 656-669 (2021).

- *Making by grinding: mechanochemistry boosts the development of halide perovskites and other multinary metal halides*. F Palazon, Y El Ajjouri, HJ Bolink, ***Adv. Energy Mat.*** *10 (13)*, 1902499 (2020).



3

Highlighted Projects

ERC GRANTS

ERC CONSOLIDATOR

Smart Coordination Polymers with Compartmentalized Pockets for Adaptive Guest Entrance (S-CAGE)

GUILLERMO MINGUEZ ESPALLARGAS
Group: CEL

2017 - 2023

ERC STARTING

Automatized Catalysis and Single-Carbon Insertion (single-C)

ABRAHAM MENDOZA VALDERREY
Group: SOC

2017 - 2023

ERC STARTING

Chemistry and Interface Control of Novel 2DPnictogen Nanomaterials (2D-Pnictochem)

GONZALO ABELLAN SAEZ
Group: 2D-Chem

2018 - 2023

ERC STARTING

Electrical control of magnetism in multiferroic 2D materials (EMAGIN2D)

EFRÉN NAVARRO MORATALLA
Group: CRISOL

2018 - 2023

ERC ADVANCED

Molecule-induced control over 2D Materials (Mol-2D)

EUGENIO CORONADO
Group: RTMM

2018 - 2024

ERC ADVANCED

Hetero-structures for Efficient Luminescent Devices (HELD)

HENDRIK JAN BOLINK
Group: MOED

2019 - 2024

ERC CONSOLIDATOR

Metal-Organic Frameworks as Chemical Reactors for the Synthesis of Well- Defined Sub- Nanometer Metal Clusters (MOF-reactors)

EMILIO JOSÉ PARDO MARÍN
Group: MUPOMAT

2019 - 2024

ERC CONSOLIDATOR

Bringing Nanospace to Life by Adapting Pore Environments to Chemical Complexity (LIVINGPORE)

CARLOS MARTI GASTALDO
Group: FUNIMAT

2022 - 2026

ERC STARTING

Chemical Design of Smart Molecular/2D Devices for Information Technologies (2D-SMARTiES)

JOSÉ JAIME BALDOVÍ JACHÁN
Group: 2DSmartMat

2022 - 2027

PROOF OF CONCEPT

PROOF OF CONCEPT

Anion Exchange Membrane Water stack based on Earth Abundant 2D Materials for Green Hydrogen Production (2D4H2)

Coordinator: GONZALO ABELLAN SAEZ
Group: 2D-Chem

2023 - 2024

PROOF OF CONCEPT

Titanium Organic Framework Membranes for CO 2 Capture (PORECAPTURE)

Coordinator: CARLOS MARTI GASTALDO
Group: FUNIMAT

2023 - 2025

PROOF OF CONCEPT

Dry-processing of metal halide Perovskites into thin films (Aperitif)

Coordinator: HENDRIK JAN BOLINK
Group: MOED

2023 - 2025

Other European projects

QUANTERA ERA-NET

Scaling Up quantum computation with MOlecular spins (SUMO)

EUGENIO CORONADO
Group: RTMM

2019 - 2021

FET OPEN

FAult Tolerant MOLecular Spin processor (FATMOLS)

EUGENIO CORONADO
Group: RTMM

2020 - 2023

FET OPEN

Selectively activated INFOrmation technology by hybrid Organic Interfaces (SINFONIA)

EUGENIO CORONADO
Group: RTMM

2021 - 2025

Pathfinder

Single Molecule Nuclear Magnetic Resonance Microscopy for Complex Spin Systems (4D-NMR)

EUGENIO CORONADO
Group: RTMM

2022 - 2025

Research and innovation action (RIA)

Development of perovskite-Si tandem photovoltaics (NEXUS)

HENDRIK JAN BOLINK
Group: MOED

2022 - 2025

Research and innovation action (RIA)

Perovskite solar cells with enhanced stability and applicability (VALHALLA)

Coordinator: HENDRIK JAN BOLINK
Group: MOED

2023 - 2025

Innovative Training Networks (ITN)

Dry production routes for large-area benign metal halide perovskite solar cells (PERSEPHONe)

Coordinator: HENDRIK JAN BOLINK
Group: MOED

2021 - 2025

Marie Skłodowska-Curie (MSCA)

Defective Titanium Metal-Organic Frameworks (DefTiMOFs)

CARLOS MARTI GASTALDO
Group: FUNIMAT

2019 - 2021

Marie Skłodowska-Curie (MSCA)

Addressing the challenges of high-performance solution-processed OLEDs using sustainable materials (TADFsolutions)

HENDRIK JAN BOLINK
Group: MOED

2022 - 2026

Marie Skłodowska-Curie (MSCA)

Modelling spin-phonon coupling in hybrid molecular/2D materials (SpinPhononHyb2D)

JOSÉ JAIME BALDOVÍ JACHÁN
Group: 2DSmartMat

2023 - 2025

Marie Skłodowska-Curie (MSCA)

SPIN-CROSSOVER

EUGENIO CORONADO
Group: RTMM

2023 - 2025

National Networks

AM@ESP
Advanced materials in Spain

Advanced Materials Complementary Plan

www.materialesavanzados.es
National and Regional Coordinator: Eugenio Coronado
Funded: European Union NextGenerationEU (PRTR-C17.I1)

2022 - 2025

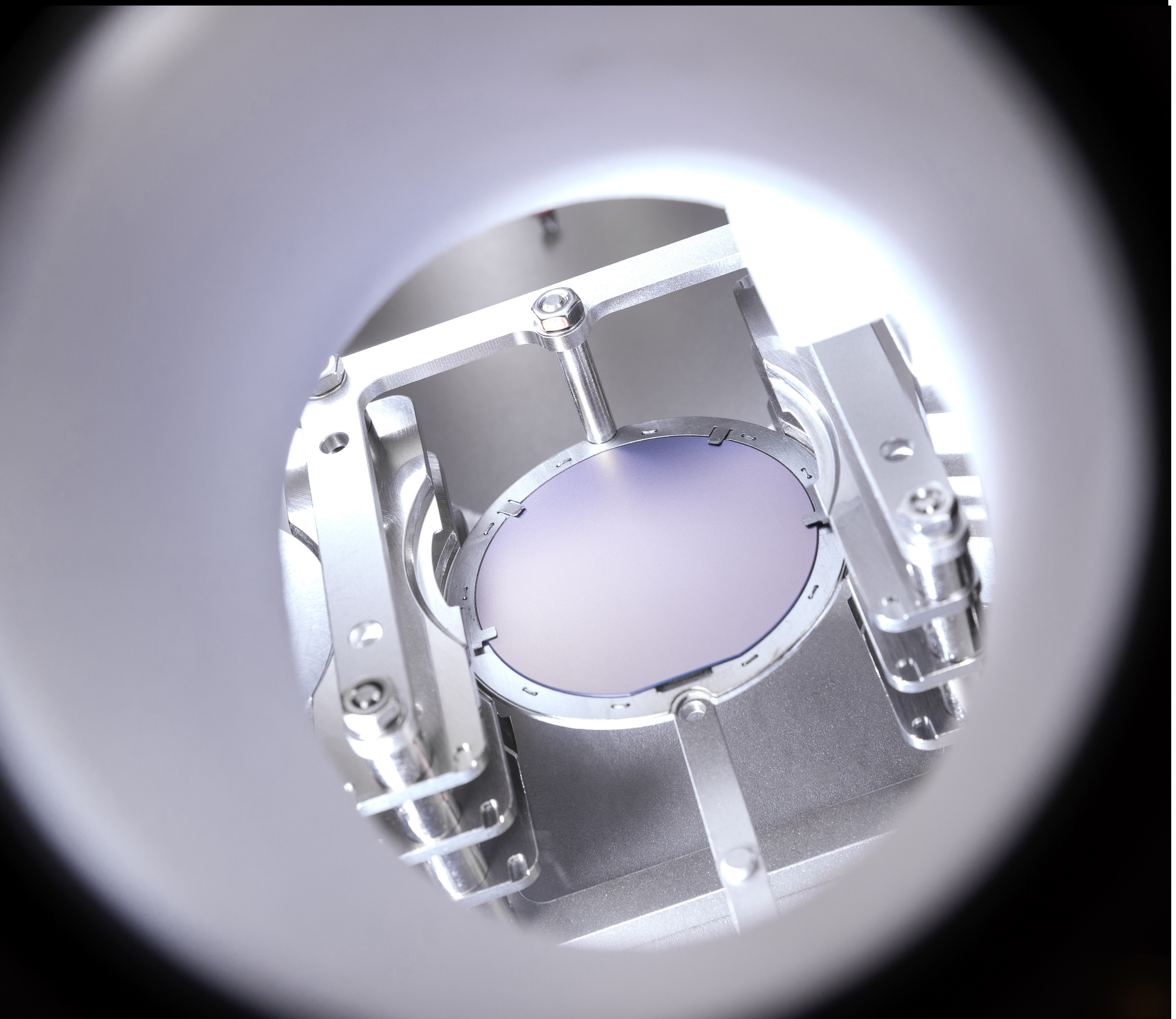
Plan Complementario de
Comunicaciones Cuánticas

Quantum Communication Complementary Plan

www.quantumcommunicationsspain.eu
National Coordinator: Vicente Martín
Regional Coordinator: Josep Capmany
Funded: European Union NextGenerationEU (PRTR-C17.I1)

2022 - 2025

4
Training & Recruitment



DOCTORATE & POSTDOC 'LA CAIXA' (2018-2023)

Fundación "la Caixa"

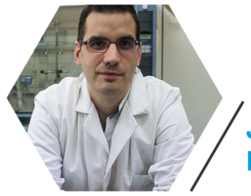
2018


Gonzalo Abellán Saez
Inorganic Chemistry


Efrén Navarro Moratalla
Inorganic Chemistry

2019


Mónica Giménez-Marqués
Inorganic Chemistry


Jesús Ferrando Soria
Inorganic Chemistry

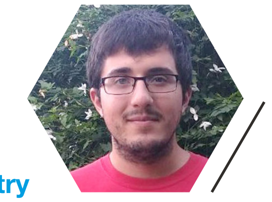

Francisco García
Technology Materials


Rosa Córdoba Castillo
Technology Materials

2020


Natalia Muñoz Padial
Organic Chemistry


Javier Segarra Martí
Physical Chemistry


Javier Carmona (Ph.D.)
Physical Chemistry

2021


Marta Galbiati
Solid state physics

2022


Filippo Mione (Ph.D.)
General Physics

2023


Isabel Abánades
Inorganic Chemistry

Ramón y Cajal Program (2018-2023)

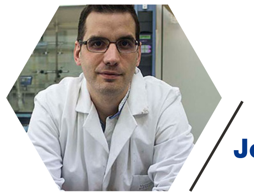
2018


Michele Sessolo


Sergio Tatay

2019


Juan Aragó


Jesús Ferrando Soria

2020


Efrén Navarro Moratalla

2021


Mónica Giménez-Marqués


Cristina Roldán

2022


Rosa Córdoba Castillo

2023


Natalia Muñoz Padial


Isabel Abánades

2023


Salvador Cardona

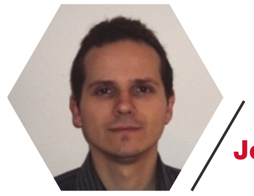
GENERALITAT VALENCIANA

Plan Gen-T Generalitat Valenciana

CIDEGENT

2018


Gonzalo Abellán


Josep Canet


Jorge González

2020


Cristina Roldán

2021


Alejandro Gaita


Abraham Mendoza

2022


Amilcar Bedoya

2023


José J. Baldoví

CDEIGENT

2019


Javier Segarra

2021


Joaquín Soriano

2022


Víctor Rubio

SEJIGENT

2021


Natalia Muñoz


Rosa Córdoba

2022

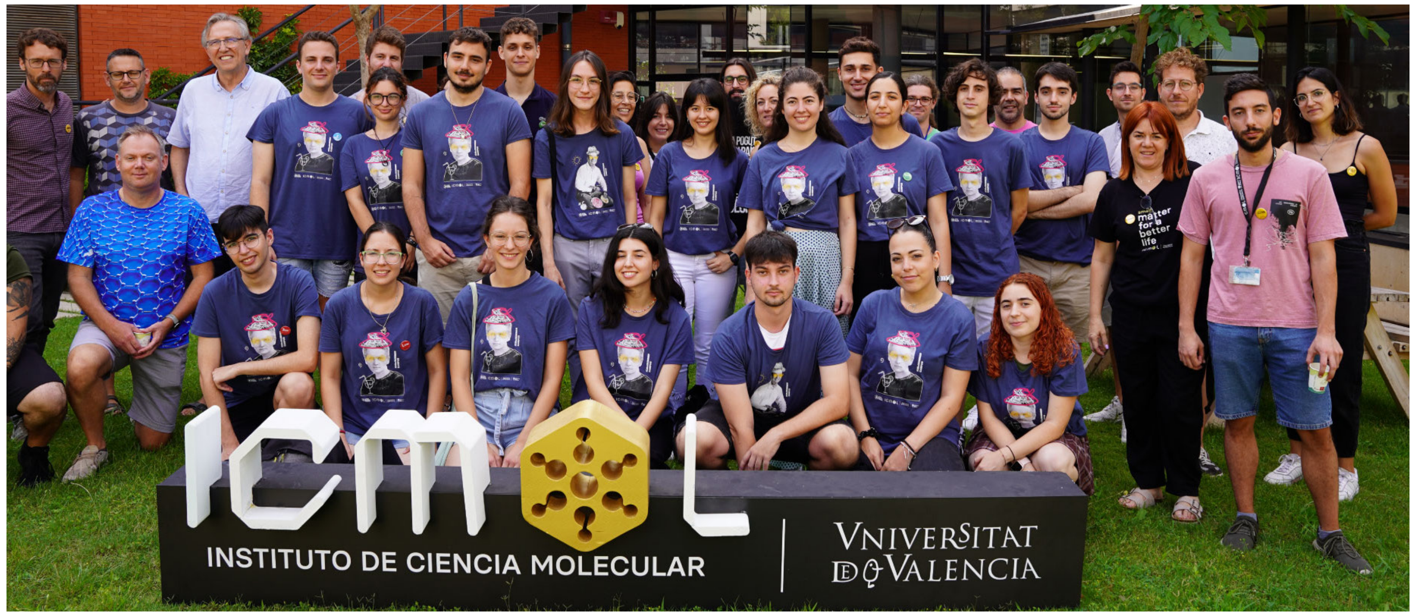

Michele Sessolo

Master & Doctorate

Undergraduate Students: ICMol Summer Campus

The Summer Campus is an ICMol initiative in which students are able to attend a series of talks about the research lines of the institute. They can get to know the different research groups of the Institute and the scientific equipment.

Living the Summer Campus is a unique opportunity to get started in the world of science in a research institute of excellence.



Who can attend?

Undergraduate students of science degrees and, in particular, chemistry, physics and engineering.

Master / Molecular Nanoscience and Nanotechnology

ICMol coordinates the interuniversity Master program in Molecular Nanoscience and Nanotechnology.This Master encompasses several disciplines: Chemistry, Physics, Engineering, Materials Science, Biochemistry, Pharmacy and Medicine.

- Interuniversity
- 60 credits (1 year)
- Access to Doctorate
- Intensive courses, in English

Goals / Master / Molecular Nanoscience and Nanotechnology

To create a multidisciplinary and competitive scientific community in Spain to research in these subjects. In this respect, the master is a suitable framework for the promotion of mobility and interaction between students from different scientific areas and contacts with other universities, research centres and companies operating in this area.
To lay down a national excellence standard in Molecular Science to empower students to research in this area or for them to gain useful knowledge and skills to be able to develop a career in high technology companies.

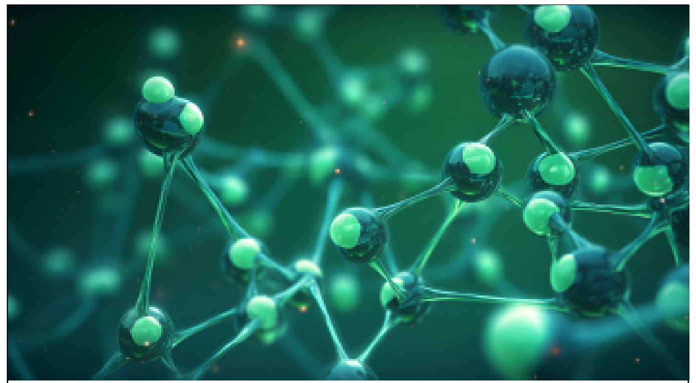
Number of students

- 2021-2022
  UV / 13 Other universities / 4
- 2022 - 2023
  UV / 15 Other universities / 25
- 2023-2024
  UV / 10 Other universities / 26

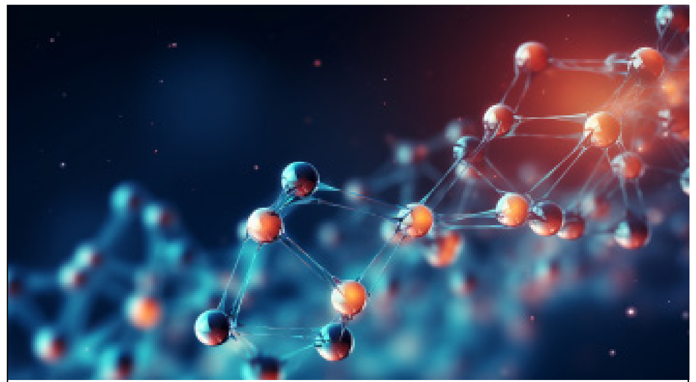
www.icmol.es/master/

VNIVERSITAT DE VALÈNCIA · UAM Universidad Autónoma de Madrid · Universitat d'Alacant Universidad de Alicante · UCLM Universidad de Castilla-La Mancha · UMH Universitas Miguel Hernández · UVa · Universidad de La Laguna

Doctorate

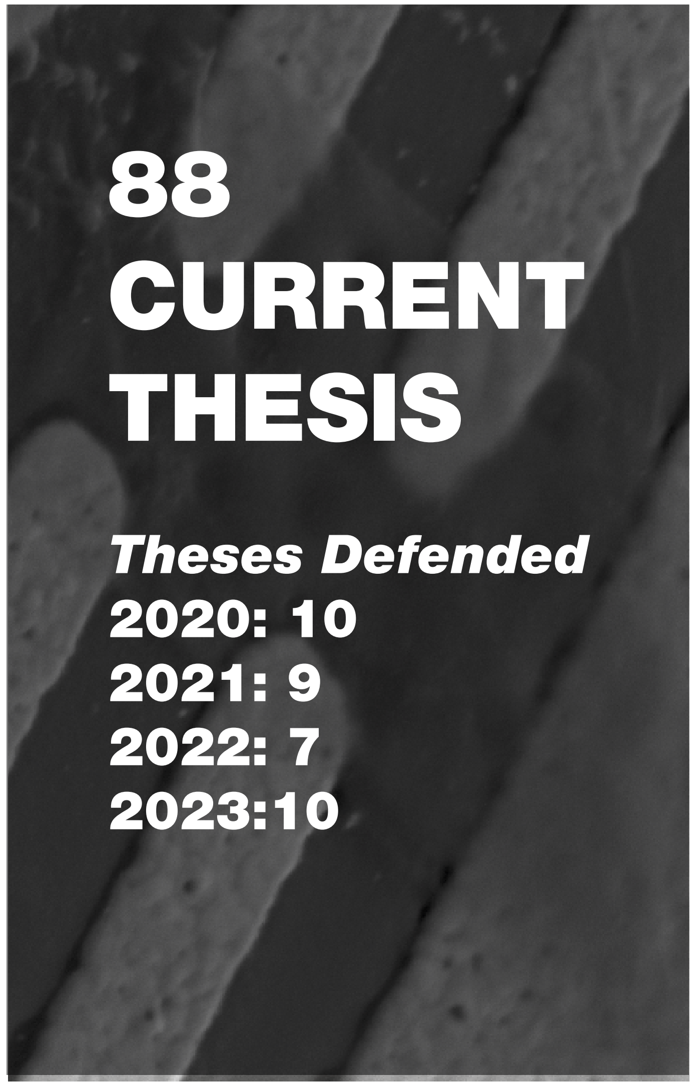


Doctoral Program in Sustainable Chemistry



Doctoral Program in Theoretical Chemistry and Computational Modelling *Erasmus Mundus*

Doctoral Program in Nanoscience and Nanotechnology



88 CURRENT THESIS

Theses Defended

2020: 10
2021: 9
2022: 7
2023:10

PhD STUDENTS

This official doctoral program was created in 2007 and received, by the Ministry of Education, the Quality Award in October 2008 (Reference MCD2008-00082) and the Excellence Mention in October 2011 (Reference MEE2011-00194). The programme is registered in the RUCT with code 5601462.

OBJETIVES

The main objective of the PhD program is the writing and defense of the PhD thesis in nanoscience.

The student must acquire a high level of professional skills in various fields, especially those requiring creativity and innovation, to cope in contexts with little specific information and to solve complex problems, as well as to design and develop novel and innovative projects.

Thus, the PhD in Nanoscience and Nanotechnology:
- Offers research training to graduates in Chemistry, Physics, Biotechnology, Chemical or Electronic Engineering, Materials Science and Technology or equivalent and to facilitate their academic, research or professional development.

- Establishes collaborative relationships with high-tech institutions and companies.

- Promotes the cooperation among different universities to develop a research profile in Nanoscience and Nanotechnology sought and recognised by the R&D sector.

Students who started their PhD at ICMol

- 2020 - 2021
  UV/13 - others/4
- 2022 - 2023
  UV/16 - others/5
- 2023 - 2024
  UV/19 - others/5

www.icmol.es/doctorado/nano

Vniversitat de València
Universitat d'Alacant
Universidad de Alicante
Universidad de La Laguna
UCLM Universidad de Castilla-La Mancha

5

Conferences and Seminars

2020

Title: Evolution in the cryptochrome-photolyase family: a computational point of view
Speaker: Natacha Gillet
Affiliation: École Normale Supérieure de Lyon - France
Date: Wednesday, January 15, 2020, 11:30h

Title: Dynamics of DNA lesions in and out the nucleosome: insights towards repair?
Speaker: Elise Dumont
Affiliation: École Normale Supérieure de Lyon - France
Date: Wednesday, January 15, 2020, 11:00h

Title: Capturing the supramolecular association of calixarenes onto proteins: the case of cytochrome C
Speaker: Alessio Bartocci
Affiliation: École Normale Supérieure de Lyon - France
Date: Wednesday, January 15, 2020, 12:00h

Title: The computing power of living systems
Speaker: Angel Goñi-Moreno
Affiliation: Newcastle University - Universidad Politécnica de Madrid
Date: Thursday, January 23, 2020, 11:00h

Title: Advances in Organic 2D Materials
Speaker: Xinliang Feng
Affiliation: Technische Universität Dresden, Germany
Date: Thursday, February 13, 2020, 18:00h

Title: Synthesis and application in organic electronics of polyheteroaromatic compounds fused with integrated pyrrole units
Speaker: David Curiel
Affiliation: Dpto. de Química Orgánica, Universidad de Murcia
Date: Friday, February 14, 2020, 11:30h

Title: Electronic and excitonic processes in organic conjugated materials. Modeling insights
Speaker: David Beljonne
Affiliation: University of Mons - Belgium
Date: Thursday, February 27, 2020, 12:00h

Title: Synthesis, characterization and modeling of magnetic nanostructures
Speaker: Juan Escrig Murúa
Affiliation: Universidad de Santiago de Chile, Chile
Date: Friday, March 13, 2020, 11:30h

Title: Molecular materials and electrochemistry for bioreplication
Speaker: Toribio Fernández Otero
Date: Tuesday, December 01, 2020, 12:00h

2021

Title: Energy transition is not only a question of physics or chemistry, but a change in our behavior
Speaker: Petra Rudolf
Affiliation: Vice-president of the European Physical Society
Date: Monday, August 30, 2021, 11:30h

Title: Cornucopia of surprises from Ag(2+), a heavier analogue of Cu(2+)
Speaker: Wojciech Grochala
Affiliation: Leader group at Center of New Technologies, University of Warsaw
Date: Tuesday, November 02, 2021, 12:00h

Title: Determining usefulness of data-driven models in materials discovery: strengths and limitations of machine learning models applied to organic solar cells discovery
Speaker: Marcos del Cueto
Affiliation: University of Liverpool
Date: Tuesday, November 30, 2021, 16:00h

2022

Title: Molecular engineering of polyoxometalates at electrodes
Speaker: Anna Proust
Affiliation: Université Sorbonne, France
Date: January 4, 2022

Title: Methods and Applications of Microcrystal Electron Diffraction (MicroED)
Speaker: Brent Nannenga
Affiliation: Arizona State University, United States
Date: April 4, 2022

Title: Inverting the singlet-triplet energy gap in triangle-shaped molecules: a matter of Symmetry and correlation
Speaker: Gaetano Ricci
Affiliation: University of Namur, Belgium
Date: April 8, 2022

Title: Host guest interactions in soft and hard matter from a computational viewpoint
Speaker: German Sastre
Affiliation: ITQ UPV-CSIC, Spain
Date: May 6, 2022

Title: Efficient and Stable Perovskite/ Silicon Tandem Solar Cells: Device concepts and stability test aspects
Speaker: Erkan Aydin
Affiliation: King Abdullah University, Saudi Arabia
Date: June 2, 2022

Title: Empty and Endohedral Fullerenes: Some Unique Structures and Properties Useful in Perovskite Solar Cells and Electrocatalysis
Speaker: Luis Echegoyen
Affiliation: University of Texas, United States
Date: June 20, 2022

Title: Intramolecular charge transfer: ab-initio calculations combined with through-space & through-bond interpretation
Speaker: Shmuel Zilberg
Affiliation: Ariel University, Israel
Date: June 22, 2022

Title: Molecular Spin Qubits for Quantum Computer and Highly Density Memory Devices Based on Molecular Magnets
Speaker: Masahiro Yamashita
Affiliation: Tohoku University, Japan
Date: July 11, 2022

Title: Conductivity and Dynamic Bonding in Nanoscale MOfs
Speaker: Karl Brozek
Affiliation: University of Oregon, United States
Date: July 29, 2022

Title: Spintronics with magnetic insulators
Speaker: Saül Vélez
Affiliation: Autonomous University of Madrid, Spain
Date: September 22, 2022

Title: Diffusion length measurements using the Steady-State Photocarrier Grating technique
Speaker: Javier Schmidt
Affiliation: Universidad Nacional del Litoral, Spain
Date: October 20, 2022

Title: Versatile Insertion-Grafting in Layered Functional Systems: From functionalization to Exfoliation
Speaker: Pierre Rabu
Affiliation: Institute of Physics and Chemistry of Materials (Strasbourg), Germany
Date: November 30, 2022

2023

Title: Superconducting diode effect due to magnetochiral anisotropy in topological insulator and Rashba nanowires
Speaker: Jelena Klinovaja
Affiliation: Universit of Basel, Switzerland
Date: February 17, 2023

Title: Chemical design for metal halide perovskites nanostructures
Speaker: Loredana Protesesku
Affiliation: University of Groningen, Netherlands
Date: March 6, 2023

Title: Reticular Nanoscience: Bottom-Up Assembly Nanotechnology
Speaker: Stefan Wuttke
Affiliation: Basque Center for Materials, Spain
Date: March 9, 2023

Title: Chemical capacitor and what it brings to chemistry and physics
Speaker: Wojciech Grochala
Affiliation: University of Warsaw, Poland
Date: March 21, 2023

Title: The New Generations of Purely Organic Emitters for OLEDs
Speaker: Jean-Luc Bredas
Affiliation: University of Arizona, United States
Date: June 9, 2023

Title: The challenge of popularizing science
Speaker: Javier Santaolalla
Affiliation: Divulgador científico, Spain
Date: June 16, 2023

Title: Topological and 2D materials grown by molecular-beam epitaxy: Synthesis and applications from the ultra-high vacuum perspective
Speaker: Amilcar Bedoya
Affiliation: Max Plank Institute of Microstructure Physics, Germany
Date: June 26, 2023

Title: Remote-controlled nucleic acids for biology and medicine
Speaker: Michael Booth
Affiliation: University College London, United Kingdom
Date: July 24, 2023

Title: Light controlling gene expression
Speaker: Sonia López
Affiliation: University College London, United Kingdom
Date: July 24, 2023

Title: Heteroatom-doped molecular graphenoids: from synthesis to properties
Speaker: Davide Bonifazi
Affiliation: University of Vienna, Austria
Date: September 2, 2023

Title: Accelerating Chemistry discovery with enhanced sampling techniques: Applications to molecular photoswitches, enzyme and heterogeneus catalysts
Speaker: Umberto Raucci
Affiliation: Italian Institute of Technology, Italy
Date: September 26, 2023

Title: Different roles of Metal-Organic Frameworks in environmental applications
Speaker: Sara Rojas
Affiliation: University of Granada, Spain
Date: October 5, 2023

Title: Design and applications of multifunctional graphene-based material
Speaker: Alberto Bianco
Affiliation: University of Strasbourg, France
Date: October 25, 2023

Title: Exploring the Invisible at the Festival of Nanoscience 10 to the minus 9
Speaker: Jordi Díaz
Affiliation: Universitat de Barcelona, Spain
Date: November 3, 2023

Title: AI and Scientific Outreach
Speaker: Pablo Escobedo
Affiliation: Prodigioso Volcán, Spain
Date: November 3, 2023

Title: How I Learned to Stop Worrying and Call It “Outreach”
Speaker: Carlos Romá-Mateo
Affiliation: Universitat de València, Spain
Date: November 3, 2023

Title: The experience of disseminating on digital platforms
Speaker: Rocío Vidal/ La gata de Srödinger
Affiliation: Divulgadora científica, Spain
Date: November 6, 2023

Title: The design of thermally activated delayed fluorescent and heavy-atom free room temperature phosphorescent supramolecular assemblies
Speaker: Eli Zysman
Affiliation: University of St Andrews, United Kingdom
Date: November 21, 2023

Title: Clip-off Chemistry; Synthesis by Bon Cleavage
Speaker: Daniel Maspoch
Affiliation: IC2N- University of Barcelona, Spain
Date: November 27, 2023

Title: Single-atom photo(co)catalysts: from hybrid DFT to the Bethe-Salpeter equation
Speaker: Piotr Blonkski
Affiliation: Palacky University Olomuc, Czech Republic
Date: December 14, 2023


Auditorio
Marie Curie &
Streaming
17/12/2021 09:00 hs
PARC CIENTIFIC
UNIVERSITAT DE VALÈNCIA
INSTITUTO DE CIENCIA MOLECULAR

6
Awards

2020

Silvia Giménez Santamarina
Entrepreneurial Potential Award
Red de Universidades Valencianas para el Fomento de la Investigación, el Desarrollo y la Innovación (RUVID)

Eugenio Coronado
Humboldt Research Award
Alexander von Humboldt Foundation

Álvaro Martínez
European Prize for the Popularization of Science
Universitat de València

Rosa Córdoba
Young Researcher Award
Micro Electronic Engineering (MEE)


Marta Mon Conejero & Víctor Rubio Giménez
Extraordinary Doctorate Award
Universitat de València

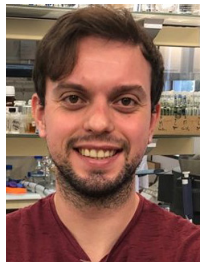
Honoris Causa Doctorate
University of Lisbon

2021

Eugenio Coronado
Forbes TOP 50 list of the most awarded Spaniards

Javier Castells
Best Doctoral Thesis
Real Sociedad Española de Química (RSEQ)

Mónica Giménez
Young Researcher Award
Real Sociedad Española de Química (RSEQ)



Javier López Cabrelles
La Ribera Scientific and Technical Prize
Ayuntamiento de Algemesí

2022

Francesc Lloret
Distinguished Career
Real Sociedad Española de Química (RSEQ)

Carlos Martí-Gastaldo
Researcher of excellence
Real Sociedad Española de Química (RSEQ)

Joaquín Calbo
Young Researcher Award
Real Sociedad Española de Química (RSEQ)

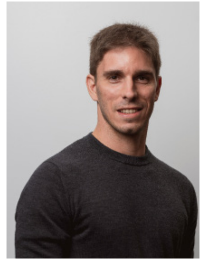
José J. Baldoví
La Ribera Scientific and Technical Prize
Ayuntamiento de Algemesí

Natalia Muñoz
Innova award
SusChem-Spain Sustainable Chemistry Technology Platform

Guillermo Mínguez
Spain's National Research Award for Young People in Chemical Science and Technology
Spanish Ministry of Science and Technology


Javier López Cabrelles
Verónica Jornet
Extraordinary Doctorate Award
Universitat de València

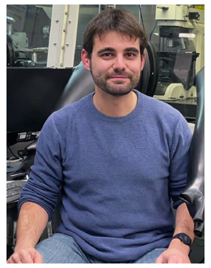
2023



Javier Castells
Extraordinary Doctorate Award
Universitat de València

Abraham Mendoza
Young researcher Award. Modality of Group Leader.
Real Sociedad Española de Química (RSEQ)

Abraham Mendoza
Young Researcher 2023
Lilly pharmaceutical & RSEQ



Samuel Mañas
Young Scientist Award
European Association of Magnetism (EMA)

Daniel Tordera
La Ribera Scientific and Technical Prize
Ayuntamiento de Algemesí

Francesc Lloret
XXIX "Estudi General" European Prize for the Dissemination of Science
Universitat de València

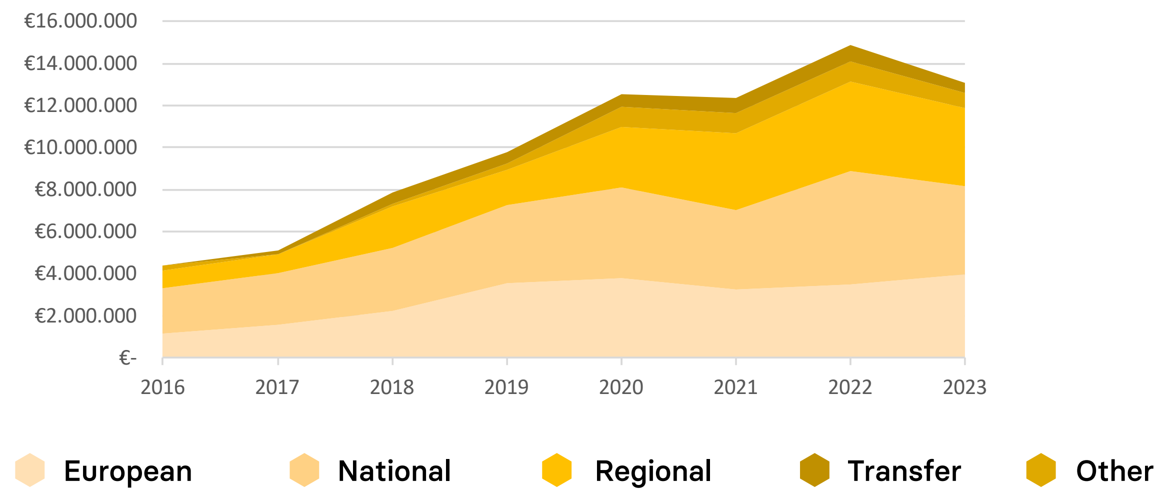
Honoris Causa Doctorate
Universidad Autónoma de Madrid

7
Funding

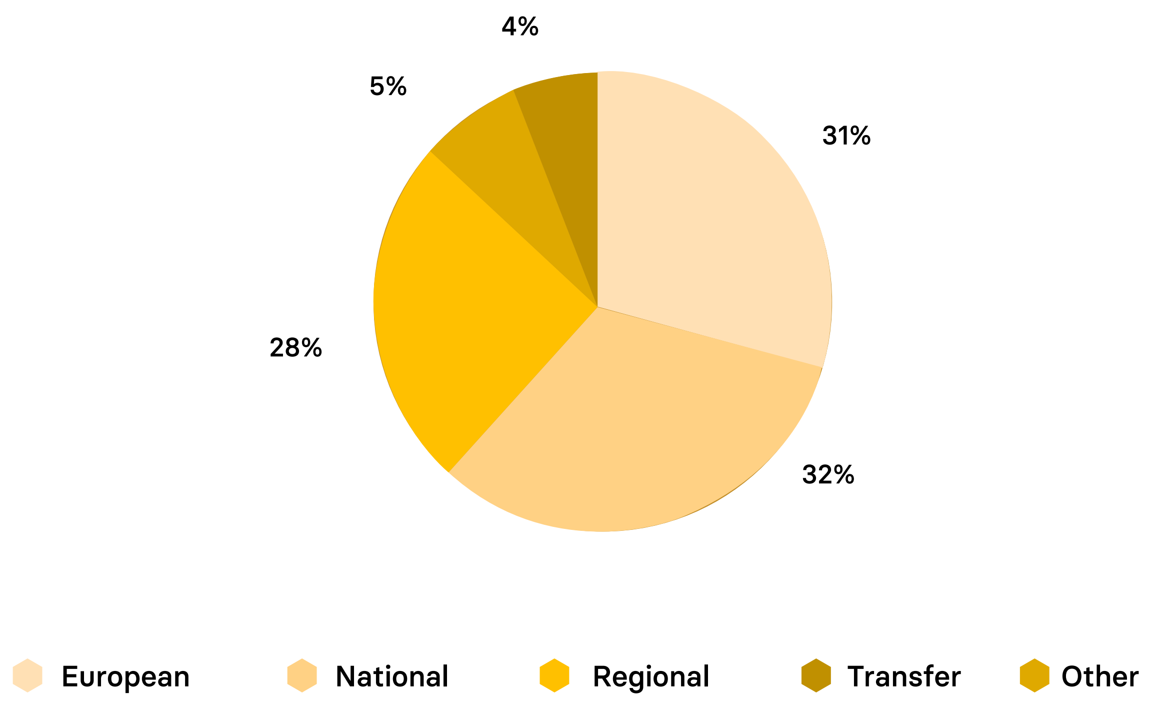
Funding

In the period 2020-2023, we have been able to attract a considerably large amount of public funds from the Regional Government, the Spanish Government, and the European Commission, and the private funding has increased.

EVOLUTION OF ICMol FINANCING OVER TIME



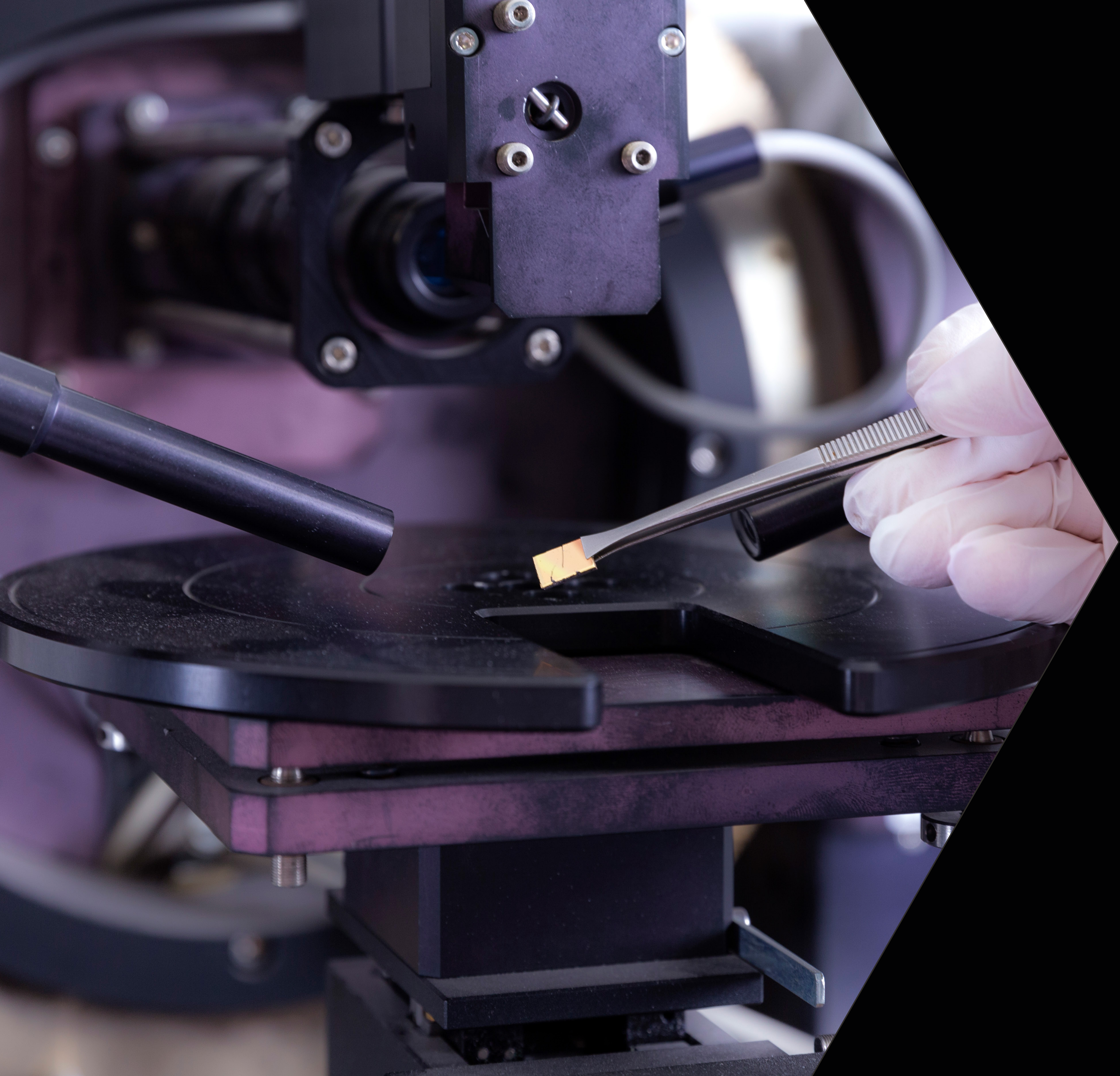
Financing 2023



PROJECTS 2023

European	3.965.562 €
National	4.079.838 €
Regional	3.614.895 €
Others*	589.153 €
Transfer	464.334 €
	12.713.781 €

* Universitat de València, Fundación la Caixa, Fundación BBVA.



8
Tech Transfer

Tech Transfer

ICMol as a Technological Partner

In recent years, and without neglecting fundamental research, ICMol has devoted to great effort and many resources bringing scientific excellence to the companies, supporting applied research and innovation. The creation of a Scientific Innovation Unit at the center, funded by the Valencian Innovation Agency (AVI) since 2018, has been a turning point in the transfer activity.

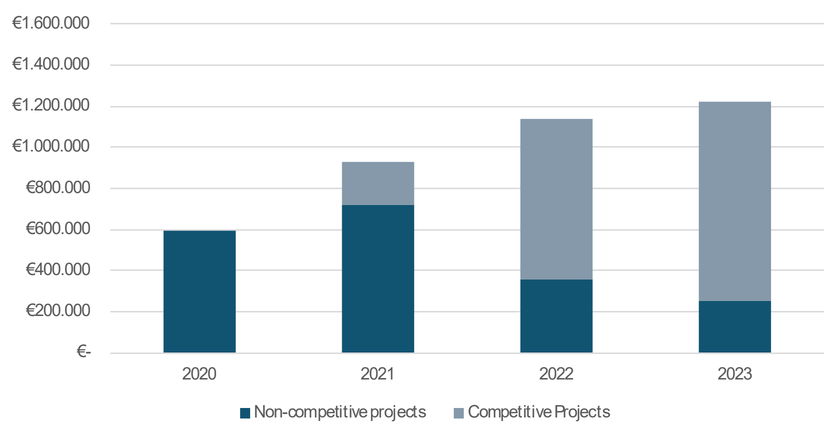
The commitment to transfer, in a centre that has traditionally been characterised by developing basic research, is a necessary challenge for the adaptation of research to the new needs of society and the market and has meant a strategic change in ICMol's research. The planning, support, guidance and training carried out has contributed not only to improve the centre's transfer figures, but also to maintain its scientific excellence.

Team

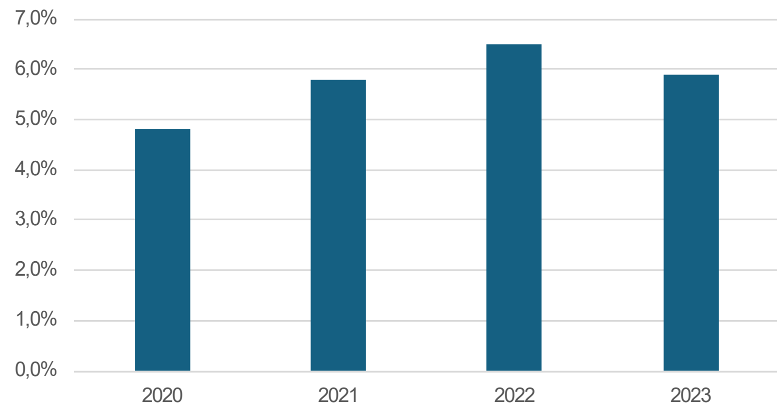
Antonio Alberola
antonio.alberola-catalan@uv.es

Francisco Marqués Guijarro
francisco.marques-guijarro@uv.es

Funding Evolution in Technology Transfer



Funding Evolution in Technology Transfer



AVI-funded projects and PROOF OF CONCEPT projects 2020 - 2023

Total amount of AVI projects awarded 2020-2023: 2.028.383 €

LDHPACK
Project Title: Development of 100% recyclable flexible barrier packaging by additive LDHs in coatings.
Amount: 208.205,04 €
AVI programme: Valorization and transfer of research results to businesses

INNOTEX
Project Title: Innovative technical fabrics for Personal Protective Equipment with improved activity against organophosphoesters Amount: 248.182,47 €
AVI programme: Valorization and transfer of research results to businesses

BIOCLEAN
Project Title: Research and development of an integrated biotechnological system for cleaning and disinfection of pathogens with application in food safety and clinical fields
Amount: 123.115,33 €
AVI programme: Strategic cooperation projects

FOTOSPINNER
Project Title: Photospinner a high-performance photoreactor for accelerated CO2 valorisation
Amount: 221.842,90 €
AVI programme: Valorization and transfer of research results to businesses

UCIE
Mantenimiento y desarrollo de una unidad científica de innovación empresarial
Amount: 1.375.000 €
AVI programme: Valorization and transfer of research results to businesses

Total amount PoC projects awarded 2020-2023: 933.000 €

MAGPAC
Project Title: High-performance hybrid magnetic supercapacitors
Amount: 115.000 €

Project Title: Adding Value to Material of Interest for LEDs and Photovoltaics
Amount: 120.750 €

Project Title: Robust LEDs in micrometric thicknesses
Amount: 117.000 €

TEXPROTECT
Project Title: Respiratory Protection Equipment with degradative activity
Amount: 143.750 €

2DBiBatt
Project Title: High-performance sodium-ion batteries based on bismuthene nanomaterials
Amount: 149.500 €

2D4H2
Project Title: Anion Exchange Membrane Water stack based on Earth Abundant 2D Materials for Green Hydrogen Production
Amount: 150.000 €

PORECAPTURE
Project Title: This Titanium Organic Framework Membranes for CO 2 Capture
Amount: 150.000 €

Aperitif
Project Title: Dry-processing of metal halide Perovskites into thin films
Amount: 150.000 €

Private Funded Projects 20/23

>30 / **No. of agreements with companies**

1,2 M € / **In Private Funded Projects**

Patents and licensing 20/23

New developments that have been protected in recent years

- Titanium-iron MOF solid, procedure of synthesis and use for detoxification purposes (P202030047)

- Polymeric membrane based on porous metal-organic frameworks for the decontamination of polluted waters (IT202000014074)

- Use of Simple Acyclic Polyamines for the Treatment of Diseases Caused by Parasites of the Genus Leishmania (P202030713)

- Method for determining the presence and/or stage of malignant tumors through a urine sample (P202130104)

- A layered double hydroxide, a process for the synthesis and uses thereof (EP21382113)

- Memristive devices based on molecular-based semiconducting polymeric materials using ionic migration phenomena (P202130383)

-
Compound Comprising Ruthenium(iii) and 2,2'-Biimidazole (Runat-Bi) and the Therapeutic Use Thereof (P202130624)
2D Anisotropic Bismuth Materials and Method for Obtaining Same Using Colloidal Synthesis (P202130722)

- Photonic device with electro-optical bistability and non-volatile behaviour at ultra-low power (P202130999)
- Process for Making Multicomponent Perovskites (EP22382235)

- Flash evaporation of perovskites (EP22382422)

- Devices and electrodes for energy storage and conversion systems are metallic collectors (ES20221008)

- Improved synthesis process of perovskite solar cells and diodes by aerosol flash evaporation (EP23382411)

- Heterometallic dimer catalyst stabilised in a metal-organic network with methylcysteine and its use in acetylene semi-hydrogenation (P202330601)

- Hybrid perovskite upconvesion materials (EP23382748)

- Use of the compound [Iron(II)(Hidrotris(3,5-Dimetil-1-Pyrazolyl) Borate)2] as a temperature sensor (P202330676)

The following patents have been licensed during the period 20/23

- Metal-Organic Titanium Heterometallic Solids, procedure for their synthesis and uses (ES201830496) : Licensed to Porous Materials in Action, S.L. (PMA) company

- Solar cell (US201916459789A): Licensed to Novaled GmbH

- A layered double hydroxide, a process for the synthesis and uses thereof (EP21382113): Licensed to Two-Dimensional Mater Chem, S.L. (2D-Match) company

- Process for Making Multicomponent Perovskites (EP22382235): Licensed to Oxford PV company

Devices and electrodes for energy storage and conversion systems are metallic collectors (ES20221008): Licensed to Graphenano Energy, S.L.

Spin-Offs

Porous Materials in Action, S.L.

- PMA, founded in 2021, aims to produce porous MOF-type materials, to make them valuable for integration into technological applications and to make them available to industry.
- The Spin-Off will help make these highly versatile and capable materials known to industry, and will also be able to collaborate with technological institutes and companies that could benefit from the potential of MOFs.
- The porosity, flexibility and chemical stability of these materials allow for the design of pores with specific sizes and chemical functions, which increase and diversify their properties, providing many possibilities for the technological development of better and more sustainable products.

Two-Dimensional Mater Chem, S.L. (2D-Match)

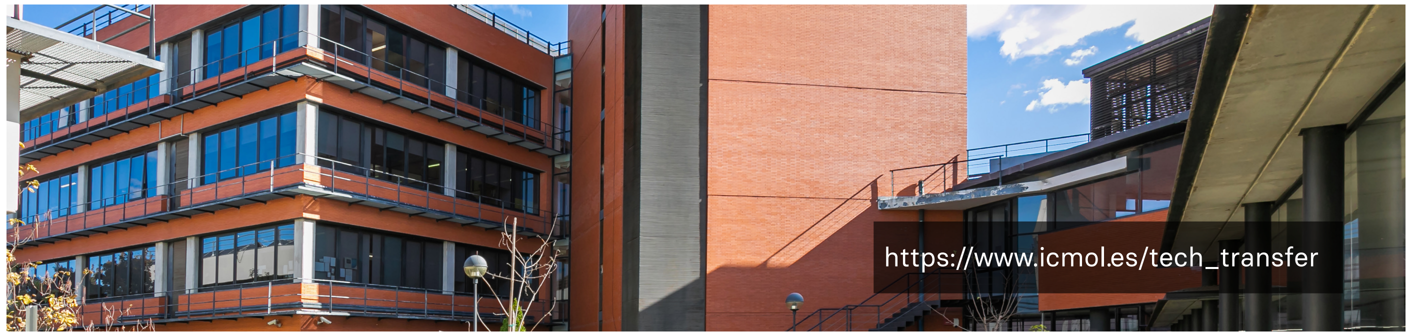
Renamed to Matteco (2023)

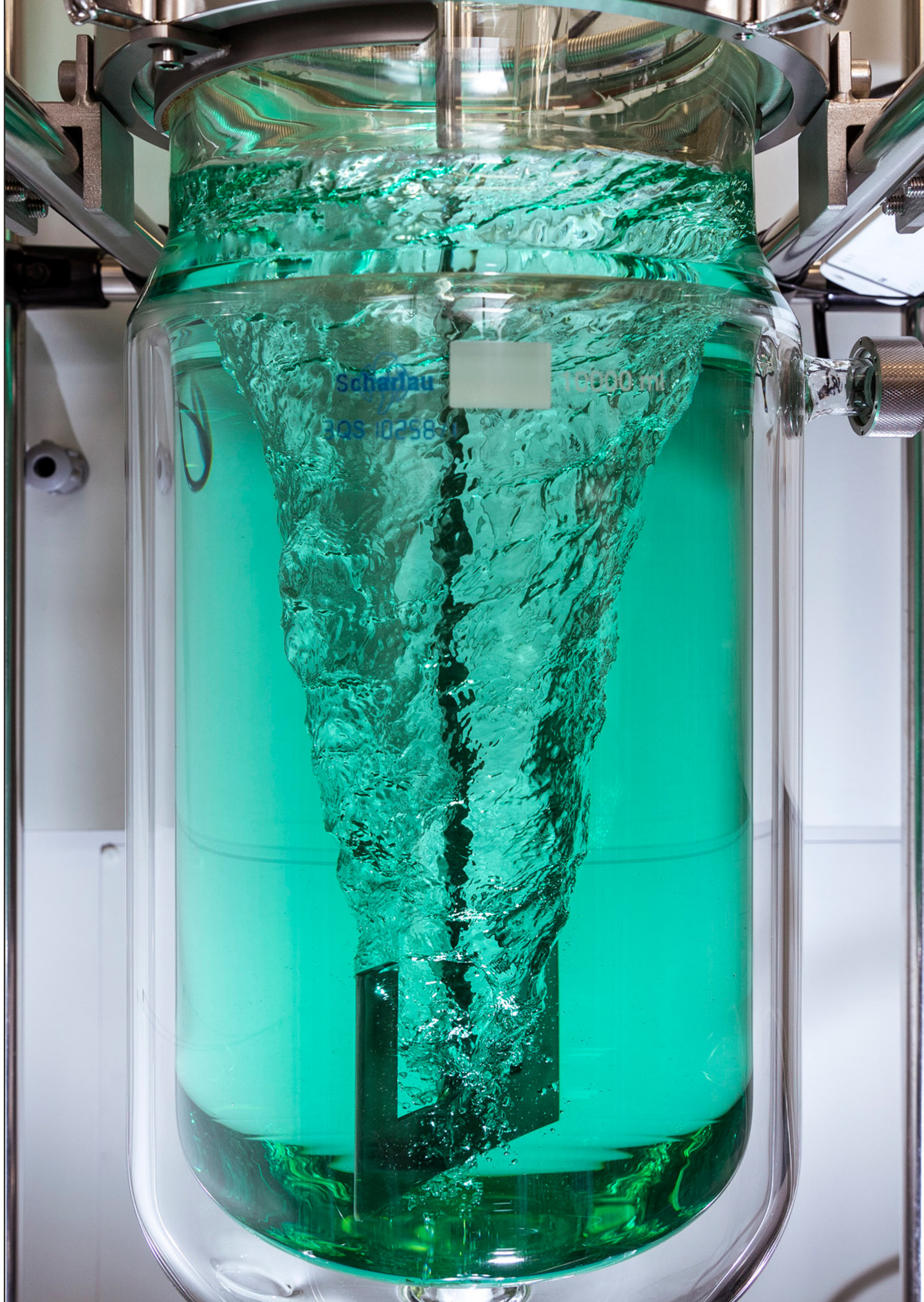
This Spin-Off was in the creation phase during 2021, and was finally founded in May 2022.

In 2023, 2D-Match had a rebranding and restructuring becoming Matteco, a company focused on the development of advanced materials for the production of green hydrogen and decarbonisation. The leap has been made thanks to the private investment of Zubi Labs.

- The Spin-Off proposes a technology capable of reducing the production costs of green hydrogen under alkaline conditions, improving its competitiveness against other types of hydrogen and other renewable energies. Moreover the technology is based on non-PGM materials.
- This technology impacts on three essential areas in order to improve the competitiveness of the water electrolysis process in the field of hydrogen production:

  1) Improvement of power-to-gas conversion efficiency (Power-to-Gas).
  2) Reduction of electrode costs (higher cost components).
  3) It allows to extend the lifetime of the electrolysers.





Maria de Maeztu Indicators

Indicator	Baseline (*)	Source and date	Expected outcomes 2023	Means of verification	Achieved results
Scientific publications of quality (D1/Q1) (Item a indicator)	163/386	Web of Science / Scopus 2015-2018	203/482	Web of Science / Scopus	226/606
International Patent Applications (PCT) (Item b indicator)	4 licensed	International Patent Applications (PCT) 2016-2019	8 applications 5 licensed	International Patent Applications (PCT)	12 applications 5 licensed
Capacity of High Level Training (Item c indicator)	43 PhD thesis	PhD Theses 2016-2019	50 PhD thesis defended	PhD Theses	36
Capacity of Recruitng Talent (item c indicator)	12 Early Career Researchers	Relevant call results 2016-2019	14 Early Career Researchers	Relevant call results	14 (9 RyC + 5 CIDEGENT)
Capacity of Recruitng Talent (item c indicator)	18 Post Doctoral Excellent Reserachers	Relevant call results 2016-2019	20 Post Doctoral Excellent Reserachers	Relevant call results	20 (6 la Caixa+ 2 cedeigent+ 10JdC+2MC)
Funding: European Projects (Item d indicator)	13.1 M €	Amount of money from competitive calls of the European Commission 2015-2018	14.4 M €	Amount of money from competitive calls of the European Commission 2019-2023	15.2 M€
Funding: European Projects (ERC) (Item d indicator)	7	Results from the ERC Grants 2015-2018	6	Results from the ERC Grants 2019-2023	7

Communication and Outreach

Communication Area

The Institute of Molecular Science (ICMol) has implemented a broad range of communication and dissemination strategies designed to promote interaction within the scientific community and with the general public. Below are the key aspects of our initiatives:

- ICMol Internal Communication: We maintain fluent and effective communication within our institute to ensure cohesion and constant updates among our team members.

Content Creation and Social Media Management: We develop relevant content and actively manage our social media profiles to enhance the visibility of our research and events.

Event/Journal/Congress Organization: We coordinate and organize scientific events, including journals and congresses, to foster knowledge exchange and collaboration among researchers.

Advice, Design, and Communication for the Various ICMol Groups: We provide support in communication and design to the various research groups at ICMol, thereby improving their visibility and recognition.

Conducting Scientific Dissemination Activities: We engage in activities to disseminate scientific knowledge to a broader audience, including talks, workshops, and demonstrations.

Online Talk Broadcasting via Streaming/Zoom/YouTube: We facilitate access to our talks and conferences through digital platforms, extending our reach to a global audience.

Constant Update of Agenda/Web/News: We keep our agenda and website updated with the latest news and events, ensuring our community is informed of all our activities.

Media Contact: We establish relationships with media outlets to expand the dissemination of our research and events.

Advertising and Disseminating Master's/Doctoral/Scholarship Programs: We promote our master's and doctoral programs, as well as scholarship opportunities, to attract talented students and professionals.

As outlined in the following pages, this summary provides a comprehensive overview of the communication and dissemination activities at the Institute of Molecular Science. For more detailed information, including the latest news related to the Institute, we suggest visiting our web agenda and news section. Here, you will find detailed descriptions of all activities, programs, and pertinent information.

www.icmol.es

Contact: comunica@icmol.es

Workshops ICMol

From the Molecular Science Institute, we organize a variety of workshops designed for people of all ages. In addition, we are involved in various activities aimed at bringing science closer to the general public, with the objective of fostering scientific vocations and increasing the visibility of our institution.

Below, we list the various workshops that the Institute's researchers often conduct at various events and schools.

Selecting Salt Shaker

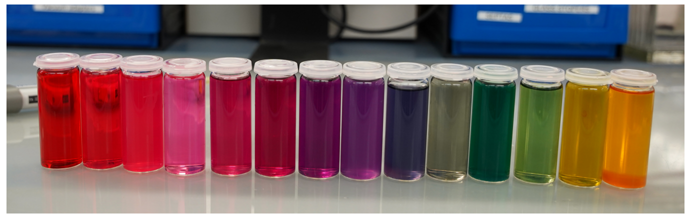
In our innovative workshop, we fuse the magic of the Harry Potter universe with real science, offering young people the opportunity to be sorted into one of the four Hogwarts houses through a unique burning salts test. This activity not only seeks to inspire scientific curiosity by observing how different salts change the colour of the flame, representing each house, but also to promote values of inclusion and teamwork, while immersing them in the exciting world of magic and science.

This methodology not only seeks to awaken interest in the chemistry and physics behind combustion and the properties of the elements, but also to foster teamwork, respect for differences and inclusiveness, core values that are fundamental to the project.

The Lombardy cabbage rainbow

In this educational and interactive workshop, we explore the fascinating world of chemistry through the "Red Cabbage Rainbow". Learn how to create your own homemade pH indicator using red cabbage, discovering the concepts of acidity and basicity in a fun and practical way. You will discover how red cabbage extract changes colour when it comes into contact with acids and bases, inviting you to experiment and have fun while unveiling the magic behind the colours.

The "Red Cabbage Rainbow" workshop demonstrates how anthocyanin pigments in red cabbage change colour with acids and bases, serving as a natural pH indicator. These colour changes, ranging from pink or red in acidic environments to blue, green or yellow in basic conditions, are the product of structural alterations in the molecules. This phenomenon illustrates the use of pH to measure the acidity or basicity of a substance, ranging from 0 to 14.



Make your own Kryptonite

One of the most fascinating activities we do is the instantaneous creation of sodium acetate crystals from a supersaturated solution, i.e. a mixture with more solute than can normally be dissolved. By introducing a crystal or a rod into the liquid, the crystals form rapidly by releasing heat. In addition, we demonstrate how some crystals can glow under a special light, similar to kryptonite, by adding a chemical called fluorescein to the mixture.

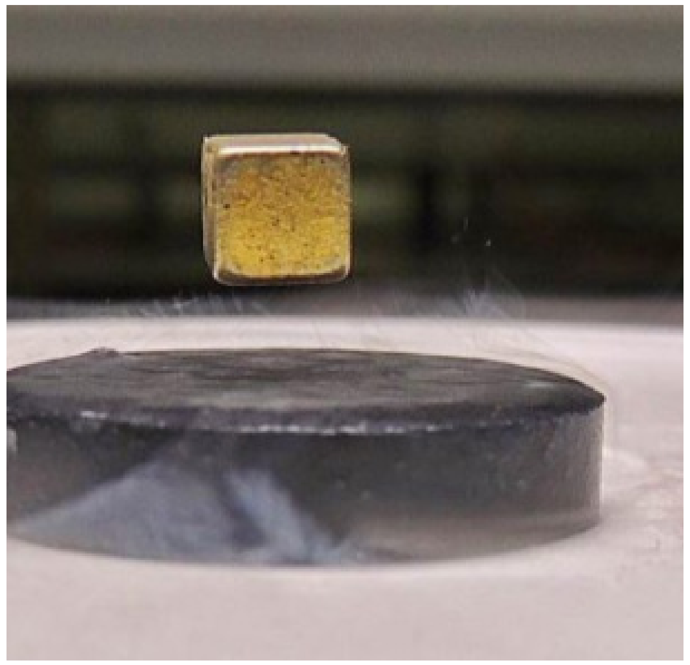
When these solutions come into contact with a crystallization nucleus, such as a rod or crystal of sodium acetate, they immediately crystallize exothermically (releasing energy, in this case heat), resulting in massive crystals instantaneously. Additionally, the demonstration aims to showcase the phenomenon of fluorescence by including small amounts of a fluorescent organic compound like fluorescein in the solutions. Consequently, under UV radiation, the formed sodium acetate crystal emits intense green light, resembling Kryptonite crystals.

Playing with chemistry and magnetism

Experiment 1: Lenz tube. This experiment demonstrates how a magnetic field is generated from an electric field. We use a copper tube with a slit to visualise the inside and two cylinders of the same size and weight: one non-magnetic and one with a neodymium magnet. Due to the induced currents, the magnetic cylinder slows down the speed of its fall, unlike the non-magnetic one.

Experiment 2: Magnetic levitation. Here, an object is held in the air solely by the action of a magnetic field, based on the principle of repulsion between two poles of equal magnetic charge. This allows the object to remain suspended in the air with proper control.

Experiment 3: Visualisation of Field Lines. By using magnetic powder and magnets, the powder is displaced revealing field lines, which are normally invisible.



The Chemistry of Slime

This ICMol activity allows us to learn about polymer science, materials chemistry, and the physical and chemical properties of materials in a fun and hands-on way. It is an exciting opportunity to explore and experiment with science while having fun creating our own blandiblue. We hope you enjoy this activity and are inspired to continue exploring the exciting world of chemistry and materials science!

The activity involves the creation of a crosslinked polymer (blandiblu) using common ingredients such as clear glue, water and borax. Food coloring is added for color and fluorescein may be added for luminescent properties under ultraviolet light.

Detail:

The polyvinyl alcohol (PVA) in clear glue is soluble in water. When mixed with borax, it forms a three-dimensional network that traps water, creating a semi-solid gel known as “slime”.

Create your own molecules

The activity consists of building molecules of varying difficulty depending on the age of the child. For the youngest children, molecules such as NaCl (common salt), EtOH (ethanol) or CH3COCH3 (acetone) will be modelled. And for older children, fullerenes and carbon nanotubes, so that the nanotube grows over the course of the workshop.

Talks and workshops in schools

At the Institute of Molecular Science, our priority is to bring science closer to young people through workshops and talks in schools. These activities are designed to awaken curiosity and interest in science from an early age, thus fostering scientific vocations.

In addition to these initiatives, we provide a special nano kit to train teachers in nanotechnology. This kit provides them with the necessary resources to effectively explain the basic concepts of this field, which is not yet widely available in school curricula. We believe it is essential to provide educators with up-to-date tools to address advanced scientific topics in the classroom.

Our goal is to contribute to the development of a more scientifically literate society that is prepared for the challenges of the future. We strongly believe in the importance of cultivating an interest in science from an early age and providing educators with the necessary resources to do so effectively.

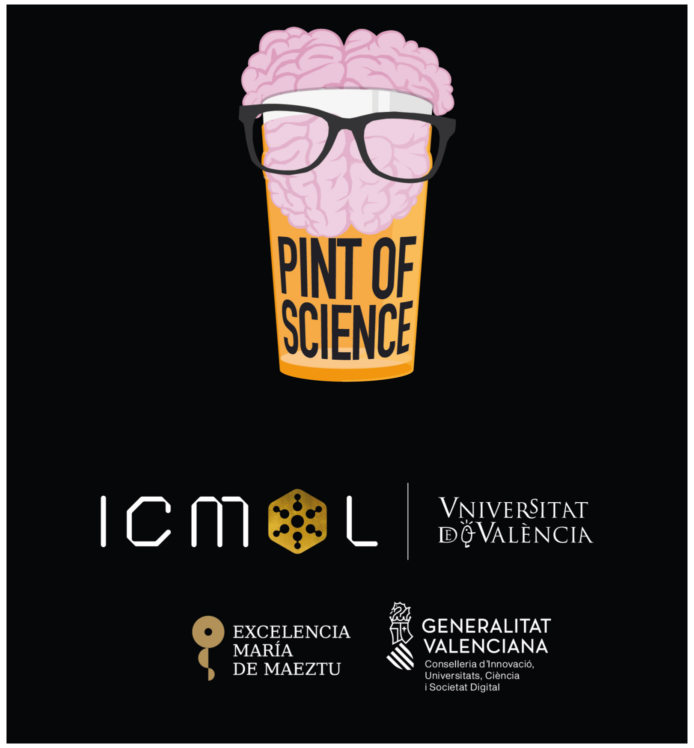
Women and Girls in Science Day

In commemoration of Women and Girls in Science Day, we held talks in schools to delve deeper into the crucial role that women have played in the scientific field. During these sessions, we explore in detail the historical and contemporary contributions of outstanding women scientists who have left an indelible mark on their respective fields of study.

We dive into the lives and achievements of pioneering women in science, highlighting how they defied gender stereotypes and overcame obstacles to achieve success in a traditionally male-dominated environment. From iconic figures such as Marie Curie to contemporary female researchers who are leading scientific breakthroughs in diverse disciplines, we look at how their work has transformed our understanding of the world around us.

Through these talks, we seek to inspire girls to follow their scientific passions and to recognize the value of their contribution to the advancement of science. In addition, we promote a reflection on the importance of gender equality in science and how recognizing and celebrating the role of women in this field is critical to building a more inclusive and equitable future.

José Rubio Malagón (@malagonadas)dedicated one of his conceptual cartoons to the Institute of Molecular Science on the occasion of #11F, International Day of Women and Girls in Science.



Pint of Science

Participation in Pint of Science (PoS)

The Pint of Science festival was born in May 2013 and aims to offer interesting, fun, important talks on the latest scientific research, in a format accessible to the public, and in a relaxed environment: a bar.

The PoS aims to bring research people closer to the public, taking advantage of the relaxed and friendly atmosphere of bars, to facilitate their interaction. In 2015 the 1st edition of PoS was held in Spain, and also in València, where since then the festival has been increasing in participation exponentially. In the 2019 edition in Spain - the second country with the most PoS venues in the world - a total of 387 events were held in 148 bars, with the participation of 784 scientists and scientists as speakers, which highlights the impact of the festival.

ICMol participated in the last editions in Valencia and intends to continue participating in future editions from its resumption in 2022.

PINT 2022

Eduardo Andrés García:
A CHEF IN THE LABORATORY

Sònia López Molina, Adriana Gil Martínez:
THE ART OF CHEMISTRY

PINT 2023

Eduardo Andrés García
FORJADO A CIENCIA

Isabel Abanados Lázaro
NANOCABALLOS DE TROYA

European Researchers' Night

The European Researchers' Night has been held simultaneously in 371 European cities since 2005. Its aim is to bring the figure of the researcher closer to the citizens so that they can learn about the impact of their work in everyday life. During the event, free, festive and fun activities take place, whose protagonists are both citizens and researchers.

La Nit de les investigadors is the Valencian version of this European festival, in which countries from all over the continent come together on a special night to disseminate science to the general public. ICMol is part of this initiative every year, participating with several workshops.

Igualment fest

Igualment Fest is a festival that aims to raise awareness and normalize gender equality from a positive artistic and social vision. A festive day framed in the International Day for the Elimination of Gender Violence in which entities and cultural and social agents, will bring the message of gender equality to the Valencian citizenship.
ICMol participated for the first time in 2018, continuing in subsequent editions.

Nanoscience Vermouth

The Nanoscience Vermuth is a series of online talks given by various national and international scientists. Below, we detail the participation of the Institute of Molecular Science (ICMol) in this series of conferences.

ICMol 2021 Talks

- “Química en dos dimensiones: cómo modificar y limpiar grafeno en la nanoescala”
  20.04.21 - 12:00h Gonzalo Abellán (ICMol)

- “El efecto espejo en la microscopía de fuerza atómica: alternativas creativas al trabajo sistemático”
  21.04.21 - 12:00h Josep Canet-Ferrer (ICMol)

- “Nanomateriales semiconductores fotoactivos ¡Chiquitos, confinados y emisivos!”
  22.04.21 - 12:00h Raquel Galián (ICMol)

ICMol 2022 Talks

- Raquel Galian - Luminescent Materials
- Camilo Jaramillo - Batteries, myths and truths.
- Eduardo Andres Garcia - Adds Gas! Save the World!
- Alejandra Soriano - X-ray Diffraction
- Alicia Forment-Aliaga - From the macro world to the nanoworldmeter

Camilo Jaramillo - Baterías, mitos y verdades.

10alamenos9 Festival Nano

Eduardo Andrés García - ¡Adsorbe Gases! Salva el...

10alamenos9 Festival Nano

Maria Simón - Energías renovables

10alamenos9 Festival Nano

Alejandra Soriano - Difracción de rayos X

10alamenos9 Festival Nano

Alicia Forment-Aliaga - Del macro mundo al...

10alamenos9 Festival Nano

ICMol 2023 Talks

- Carlos David Prado Socorro - Beyond Artificial Intelligence! Neuromorphic Chips
- Isaac Brotons Alcázar - Road to nanoscience
- María Vicent Morales - Unlocking the secrets of the nanoworld with an X-ray diffractometer

Carlos David Prado Socorro - Más Allá de la Inteligenci...

10alamenos9 Festival Nano

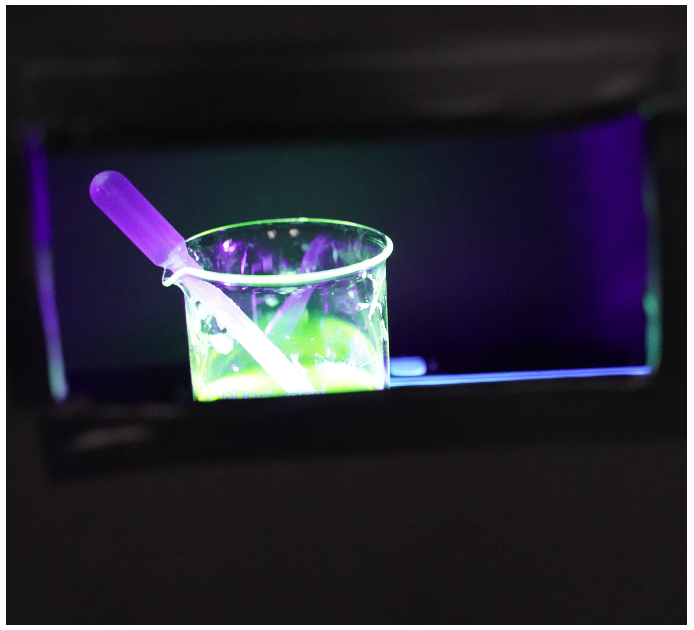
Isaac Brotons Alcázar - Camino hacia la...

10alamenos9 Festival Nano

María Vicent Morales - Revelando los secretos de...

10alamenos9 Festival Nano

EXPO CIENCIA



ICMol researchers participate in all editions of EXPO-CIENCIA, an event especially aimed at secondary schools and high schools. The University of Valencia Science Park has been organizing this annual open day for more than a decade, in which researchers and entrepreneurs of the park prepare about 60 scientific experiences, mainly aimed at the adoslescent public, children and their families.

The event allows to know, in a playful and relaxed atmosphere, the research dynamics and the scientific and business facilities of the Science Park of the University of Valencia. With activities for all ages with experiments and workshops on science and performances and attractions for children.

In the 2021 edition, after the forced break due to the Covid-19 pandemic, Expociencia was held again with the public and was attended by more than 5,000 people who visited the Science Park to celebrate the great celebration of science and innovation of the University of Valencia. Expociencia is already consolidated as one of the main initiatives aimed at sharing the scientific spirit with people and stimulating scientific vocations.

#WeAreICMol

NanoEnVideos Contest

The #NanoEnVídeos contest, organized at the level of the Valencian Community, is promoted by the Institute of Molecular Science (ICMol) in collaboration with the Unit of Scientific Culture and Innovation of the University of Valencia.

The aim of this contest is to promote in the educational community the interest in the nanoscale world, the so-called nanoworld, which, despite nanoworld, which despite its tiny size is very diverse and interesting.

Participants must upload at least one video related to one of the following topics:

- ***What is Nanotechnology?*** Curiosities of the Nanoworld: Define what Nanotechnology is in a creative and complete Nanotechnology in a creative and complete way. You can also talk about curiosities of the Nanoworld.

- ***Nanoscience in Nature and in everyday life:*** The nanoworld has always been there. That is why we propose you to talk about nanotechnology in nature or in elements of everyday life. Where can you find nanoscience.

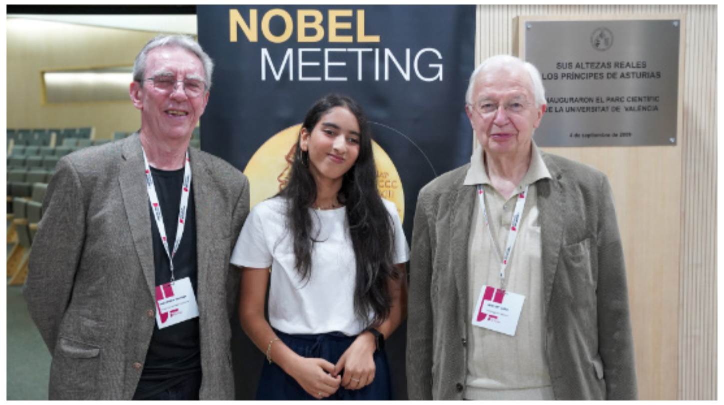
- ***Do an experiment from our Nano recipes:*** Replicate one of the experiments that we propose in the experiments that we propose in the Nano recipe book of our website.

1st Prize 2022: Maria Badau - Laura Cebriá Olivares - Lucía Domínguez Cea-cero y Miguel Ángel Giménez Banderas del @secundaria_santbertomeu

Accesit: Ximo Lloret Forment del Colegio Sagrada Familia P.J.O.

NanoStories Contest

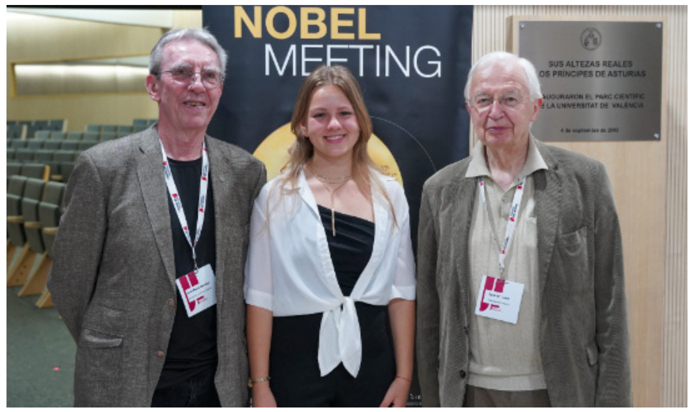
Nano relatos is a contest aimed at youngsters between 14 and 16 years in which they have to invent a short story (less tan 200 words) within the nano science topic. We aim at interesting Young students in the topic and introduce them in the classroom through an activity aimed at science and literatura teachers.



2023 / WINNERS

WINNER IN CATEGORY A 2023
Ikhlas Mansouri Mamjoud 4º ESO
IES TORRE DEL REI. OROPESA

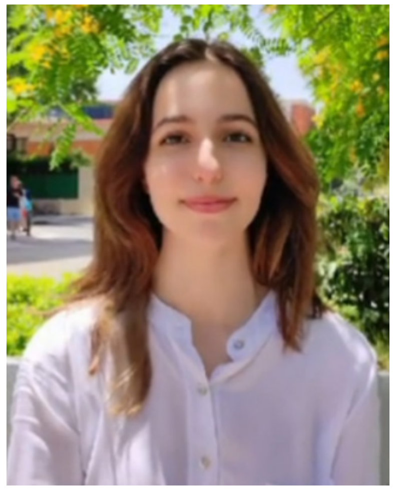
"Energy has always been a driving force in our lives, a necessary source for economic growth and improved well-being, an ability to make anything work. Energy is our lighting, our air conditioning, our electricity, our running and infinite uses. In short, energy has always been and always will be the lifeblood of our planet.
There are renewable and non-renewable energies and as you know, non-renewable energies have already retired, so they need renewable employees urgently from the International Energy Foundation. That is why I have a short interview today.
-Good morning, Mr. Hydrogen. How are you?
-Good morning, Mr. Garcia. Good, and you?
-Very well. Let's start with some questions. What can you tell me about yourself?
I am Green Hydrogen, a chemical element, very light, non-polluting, economical, inexhaustible and an energy vector.
-What benefits will we get if we hire you?
-Many, such as producing electricity, generating heat or steam, creating industrial and energetic applications, etc.
-Do you have the ability to work in a team?
-Of course, I can work with many elements and form ammonia, water, etc.
-Perfect, Mr. Hydrogen, with this information, that's enough. You are hired. You can start on Monday.
-Great, thank you very much, Mr. Garcia. "



2023 / WINNERS

WINNER IN CATEGORY B :
TO REALIZE
Nadia Júlia Rosada
1º Bachillerato. IES Rodolfo Llopis de Callosa d'En Sarrià.

"I am lying on the hospital gurney, my heart is pumping blood day after day, but less and less. I know I am slowly dying and I need someone else's heart to live. The waiting list for a match is long and most of the time, getting one in time is low.
I look to the right and find my mother praying, praying that they get to replace my heart with another one.
I look to the left and see in the distance a little park full of children my age enjoying themselves, running around, playing.
I look ahead and think that to get a heart a child like them has to die, stop living, stop creating memories and that same heart will have to become mine. A foreign heart, a heart full of memories of its past owner.
I look to the right again, and I realize that what my mother unconsciously wished for was not a new heart, but the death of a human. And with that thought alone, I decided.
I decided, at that moment, to become a nanotechnologist. So that one could receive a heart transplant without depending on the donation of another human being. To open a new era in medicine. To make what right now seems impossible a reality.



2022/ WINNERS

WINNER CATEGORY A / 2022
LA GELOSIA DELS ELEMENTS
Neus Carrascal Pastor
4º CURSO-ESO
IES CÀRCER

What jealousy, they think. The desire of every element is to become a noble gas.
all yearn with all their strength to achieve that level of constant stability that characterizes them.
they are complete, they think.
We suffer from a lack of electrons, and we do nothing but look for other elements to unite with them and appear to be noble, to be full. We are tired of so much instability, tired of changes, of constantly evolving towards any chemical formula, we feel empty, we only want to live peacefully, we feel stable.
What jealousy, they think. The desire of every noble gas is to stop being, the rest can change, they think.
change, they think. To know new elements and react with them, we are condemned to be alone, always alone.
condemned to be alone, always alone, completely alone... Our lives are
Our lives are boring, we are fed up with so much stability, with this inert life, we feel empty, we only want to see the world beyond us.

WINNER CATEGORY B / 2022
AD INFINITUM
Alejandra Ballester Lladosa
1 BACHILLERATO
COLEGIO GUADALAVIAR

The captain sighed wistfully as he checked that the required paperwork was in order. How many times had he repeated the signatures, inspected the panels and connected the machinery? He couldn't remember the exact number, but it seemed like too many. He closed the last folder authorizing the tedious process and gazed from his booth at the bleak landscape stretching out before him. A massive sphere reflected the rays of the nearest star, giving it a metallic sheen that revealed its nature: an imperfect machine, as his superiors had dictated.
Mankind had tried countless times to construct a habitat suitable for its existence, but every trial failed. Although science had developed almost magical artifacts - nanomachines they called them - with infinite uses to aid in such a mission, the current generations were already giving up on what they considered futile actions and becoming accustomed to life in spaceships.
The red button he had pressed so many times gleamed again, tempting him and warning him that it would not be their last encounter. The captain, restless, pressed the button and millions of nanomachines that made up the planet spun on themselves, beginning the end of that artificial Earth. Minutes later, his gaze reached infinity. His work was finished.

In 2022, the winning participants in the Valencian Community also took first place in the national category.

2021/ WINNERS

WINNER CATEGORY A / 2021
José Fresneda Sánchez (Cristo Rey de Benifaió).
UN TRANSPORTE DIMINUTAMENTE ENORME

The breeze comes peacefully through the hospital window, the acacia leaves sway gently in the wind, Esmeralda is lying on her bed. From between her white sheets, different pathways emerge, keeping her constantly monitored. She is undergoing a revolutionary treatment against cancer, she represents the hope of nanoscience.
But, let's get to the point, our protagonist, a small amount of everolimus, anti-cancer medicine, is heading towards her pancreas, it needs to be transported. That's where nanoscience comes in, a meticulously formed microparticle will be the transport.
It enters the bloodstream and the first problem arises. The fast-moving red blood cells are hard at work transporting oxygen to the human body. However, they have guardians, white blood cells, larger in size, which are dedicated to eliminating threats. The microparticle, assimilating the strategy of some viruses and bacteria, adapts its physicochemical structure to pass through the control of these its stowaway, the everolimus cargo.

Iberoamerican Meeting of Nanodivulgation 2023

The 5th Ibero-American Nanodivulgation Meeting, held on November 2nd and 3rd, was jointly organized by the Institute of Molecular Science (ICMol), the “10alamenos9” Festival, and the Scientific Park of the University of Valencia. This event was designed to promote knowledge and dissemination in the field of Nanoscience through a program that included talks and workshops aimed at diverse audiences, from students and teachers to the general public.

Highlighted Speakers

Rocío Vidal (@lagatadeschrodinger): The science communicator and journalist stood out for sharing her experiences in scientific dissemination through social media, demonstrating the importance of digital communication today.

Pablo Escobedo: An expert in the use of Artificial Intelligence for communication, he provided a practical perspective on leveraging these technologies in scientific dissemination.

Carlos Romà-Mateo: The biochemist and PhD in Molecular Biology and Genetics addressed the topic of scientific communication as a profession, highlighting the challenges and opportunities in the field.

Activities and Workshops

Nanotechnology Training for Teachers: Led by Jordi Díaz, PhD in Chemistry, this workshop focused on providing Science teachers with practical strategies and tools for teaching Nanoscience, introducing the “Nanokit” as a didactic resource.

This meeting not only served as a platform for the dissemination of scientific knowledge but also as a meeting point for the community interested in Nanoscience, underscoring the relevance of scientific communication and education in today’s society.

Image of the broadcast programme

Iberoamerican Meeting of Nanodivulgation 2023

Javier Santaolalla visits ICMol 2023

Santaolalla, originally from the Canary Islands but born in Burgos in 1982, and considered one of the most important science communicators in the Spanish-speaking world, led a talk on June 16 at the Marie Curie Auditorium of the University of Valencia Science Park, organized by the Institute of Molecular Science (ICMol). The event attracted a diverse audience that included physics and chemistry students, aspiring engineers, professors, and researchers, men and women of various ages, from young to old, and the occasional teenager who managed to secure one of the coveted spots for the event with the renowned YouTuber.

This gathering did not follow the conventional format of a conference; it lacked a title or a specific theme, allowing Santaolalla not only to explain scientific aspects but also to share details about his career, which he describes as that of an exceptional, almost obsessive student who was swept away by his "madness" and "impulsiveness" to eventually abandon his research career. He first flirted with comedy and then built a real fan club fascinated by his enthusiastic way of explaining complex physical phenomena.

The event began with an informal chat between the well-known particle physicist and José Jaime Baldoví, PhD in Chemistry and distinguished researcher of the Gen-T Plan of the Generalitat de Catalunya at ICMol. Baldoví and Santaolalla shared reflections on how education should "communicate" with students and about the "social" role of scientific dissemination. This exchange of ideas led to a lively discussion with the audience, where Santaolalla's comments provoked interventions full of curiosity. The discussion lasted over an hour and a half, with Santaolalla highlighting that "curiosity runs in our veins, it is what makes us feel human, but at the same time it encourages us to be scientists."

Communicator and "Artist"

Santaolalla declares himself a communicator and "artist". He often says that his vocation to bring science closer to society came after reading Stephen Hawking's book "A Brief History of Time". When asked about the emotion he brings to his interventions, Santaolalla compared his work to that of a child "for whom everything is new" or that of a superhero "who tries to go beyond his own senses." And he stated that everyone can be a superhero in their own way.

Activities for researchers

At the Institute of Molecular Science (ICMol), we conduct activities specifically targeted towards researchers, among which the following stand out. These activities not only foster dialogue and knowledge dissemination within the scientific community but also promote interaction among different actors in the academic and professional fields.

Nobel Colloquiums (#NobelMeeting):

A colloquium promoted by the Rei Jaume I Awards Foundation, in collaboration with the Institute of Molecular Science (ICMol) and the Parc Científic of the University of Valencia. In these events, laureates of this prestigious award, usually in the field of Chemistry, engage in an informal dialogue with the audience, comprised of researchers, students, professors, and other professional profiles from the academic realm.

Scientific Conferences:

In what has become a tradition since its foundation, the Institute of Molecular Science (ICMol) at the University of Valencia organizes its annual Scientific Conference. This event, the most important open-door act of the year, concludes with the contributions of prominent national and international scientific personalities and a high-level debate on current issues related to scientific activity.

Seminars:

Talks given by invited researchers, which currently, due to high demand, many of these talks are also streamed online.

Social Media

Social Media

@icmol 2687 Followers

In our results presentation, we wish to highlight the significant impact and reach achieved through our Instagram presence at the Institute of Molecular Science. This platform has allowed us to open a window to our community and activities, facilitating interaction not only with the general public but particularly with university students.

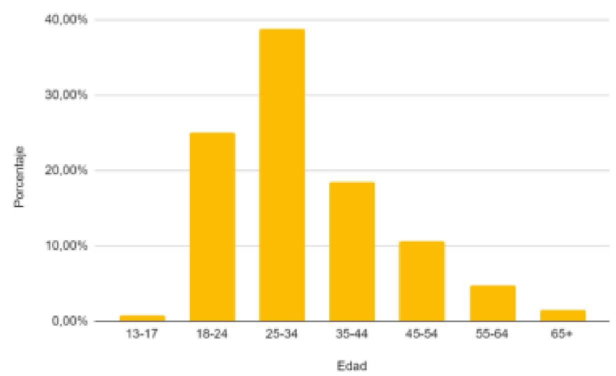
Our Instagram profile serves as a showcase to present the latest developments in molecular nanoscience and to highlight the unique atmosphere that characterizes our Institute. From showcasing the latest research to sharing more informal moments in our laboratories, our Instagram offers an intimate glimpse into our daily life.

The purpose of our activity on this social network goes beyond merely informing; we aim to immerse our followers in the Institute's universe, encouraging them to follow our activities with curiosity and admiration.

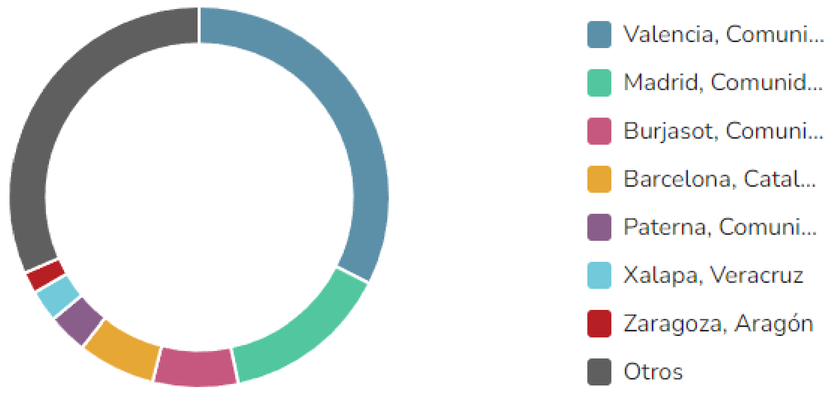
Instagram followers by age:

38.79% of followers (n=888) correspond to the 25-34 age group, followed by the 18-24 age group, which constitutes 25.01% (n=572) of the audience (Figure 12).

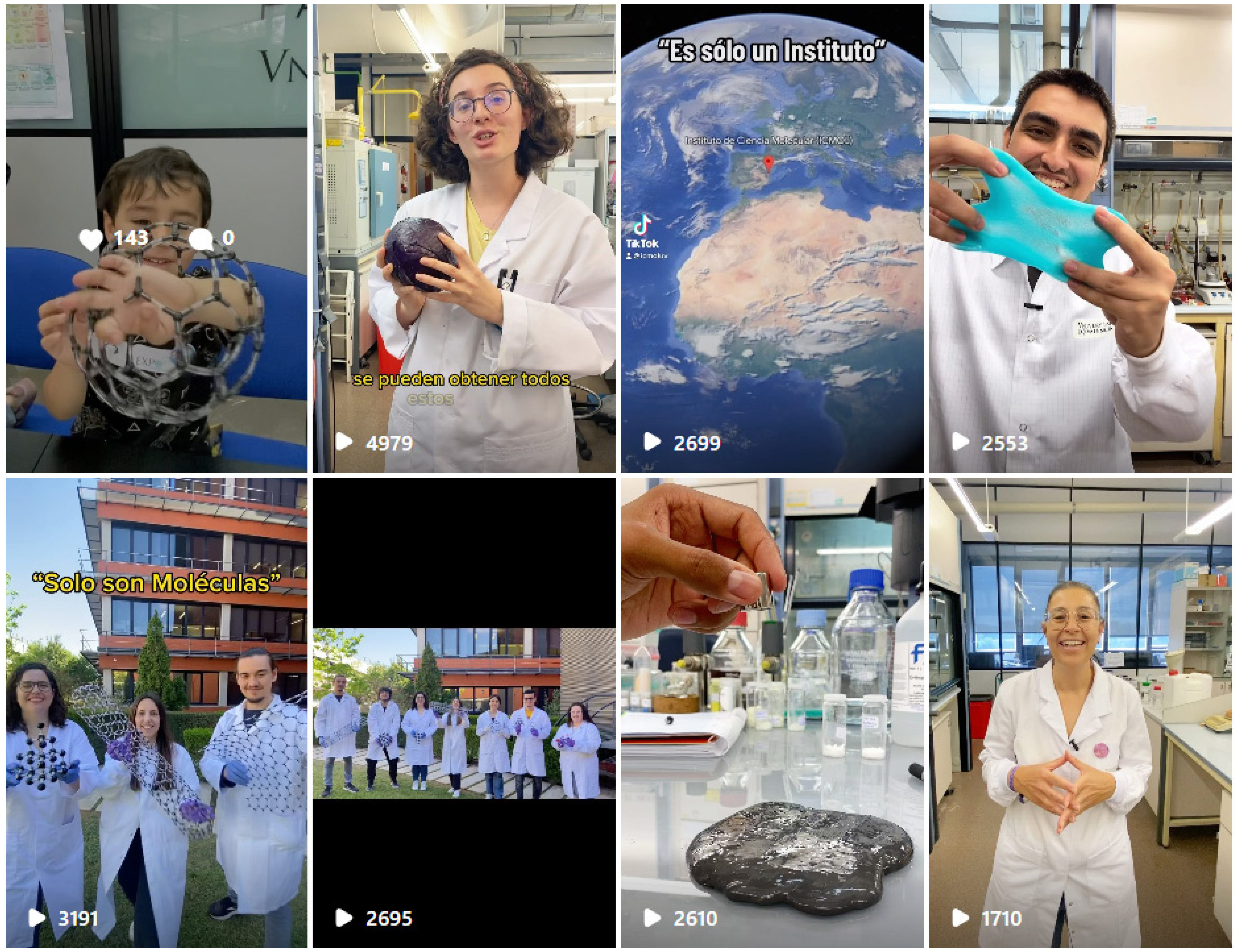
Figura 12. Seguidores de Instagram por edad



Instagram followers by region / Spain



Our online community has exhibited significant interest in our posts, as evidenced by the number of likes, comments, shares, and other interaction metrics. This level of engagement serves as a testament to the value our content delivers to our audience, as well as our ability to effectively connect with them.



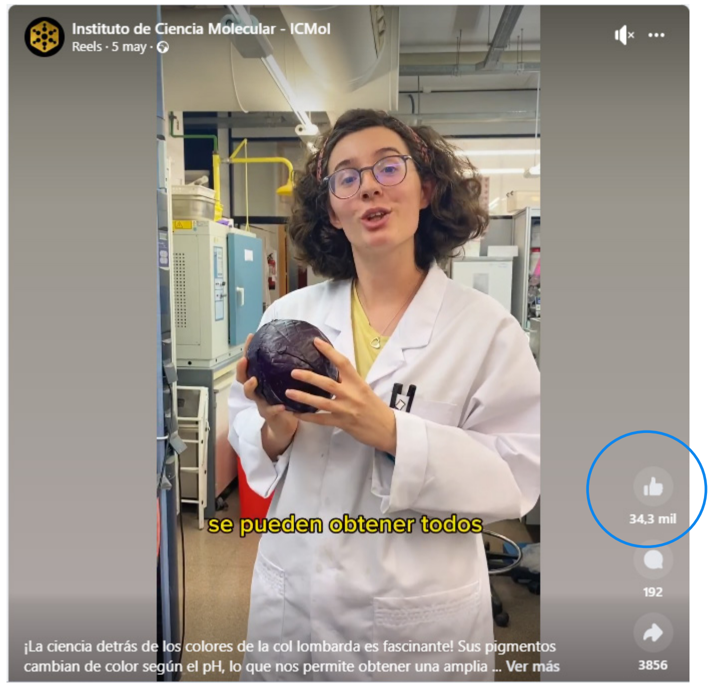
Social Media

@icmol
40.472

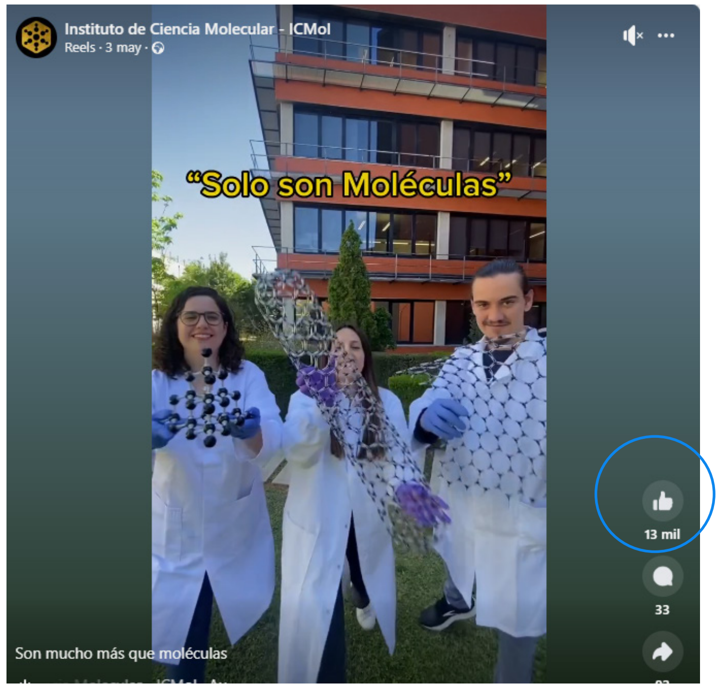
In Facebook we have gathered over 40 thousand followers, largely due to the viral spread of videos focusing on magnetism. What makes these results even more significant is that they have been achieved organically, lending additional value.

The virality of these videos signals a strong resonance with our audience, sparking their interest and encouraging them to engage with our content. This organic growth underscores the relevance and appeal of our material, proving its effectiveness in reaching and captivating a wide audience.

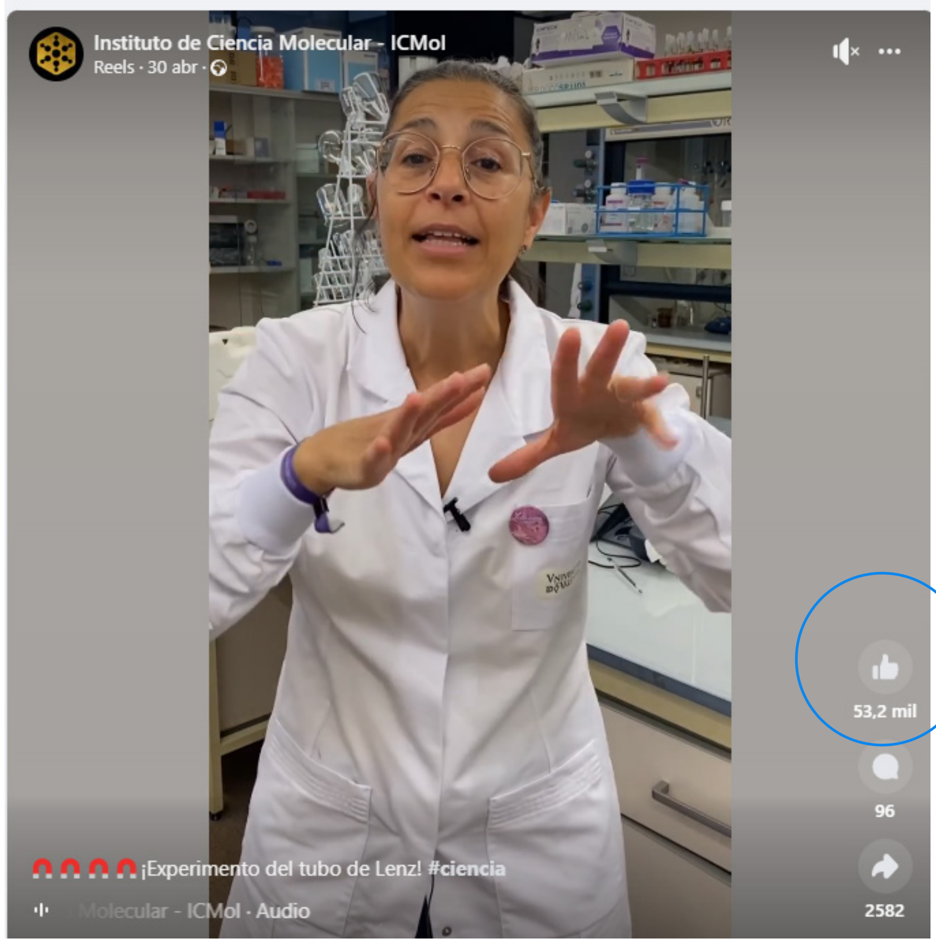
Looking ahead, we will continue to capitalize on this success by creating and sharing compelling content that stimulates curiosity, encourages engagement, and strengthens our presence within the scientific community and beyond.



34.000 Likes!

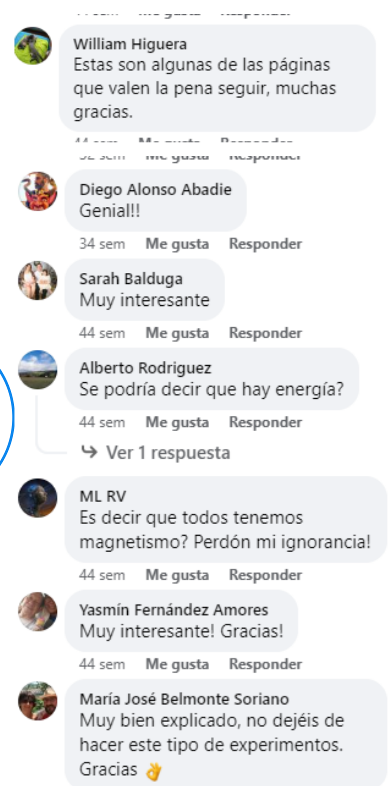


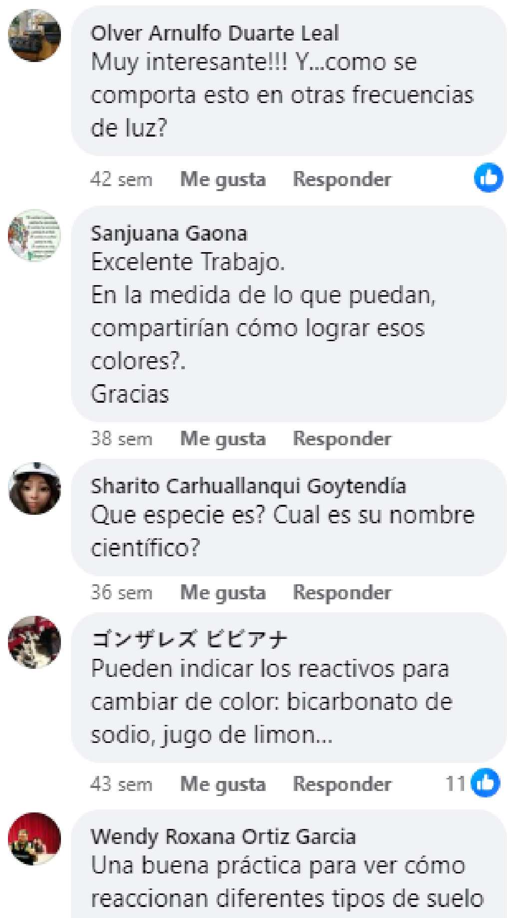
13.000 Likes!

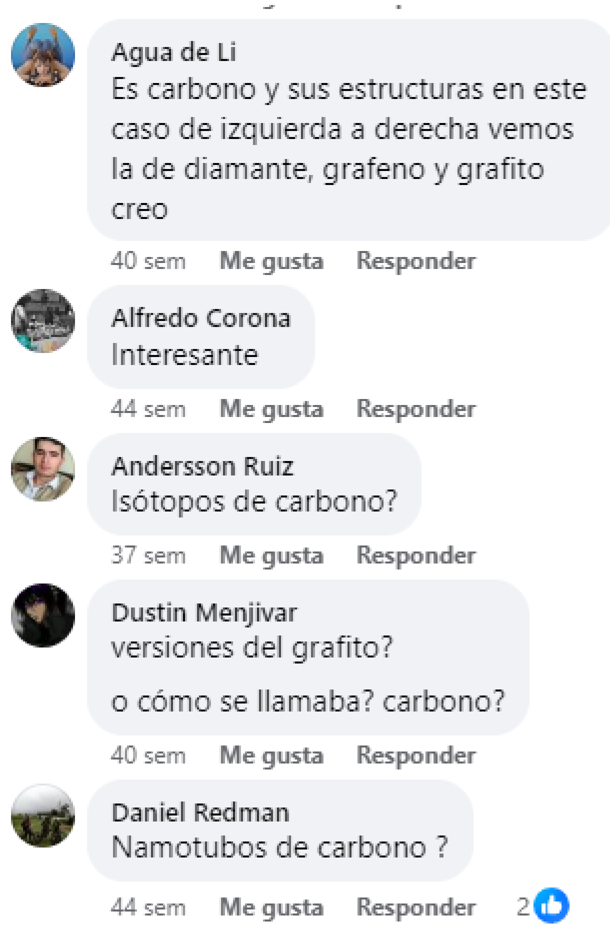


#viral

53.000 Likes!







Social Media

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2895

People

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On Twitter, we focus on sharing the advances of our research, highlighting the main investigations conducted by our scientists. Additionally, we promote the talks given by guest researchers at ICMOL and participate in relevant congresses and conferences within the field.

We also use this platform to provide an insider's view of the day-to-day activities at the institute, sharing moments and initiatives that reflect our daily work and the atmosphere at ICMOL. Our presence on Twitter allows us to keep our audience updated on our projects, events, and contributions to the field of molecular science.

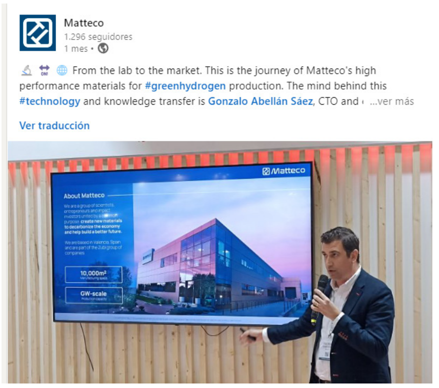
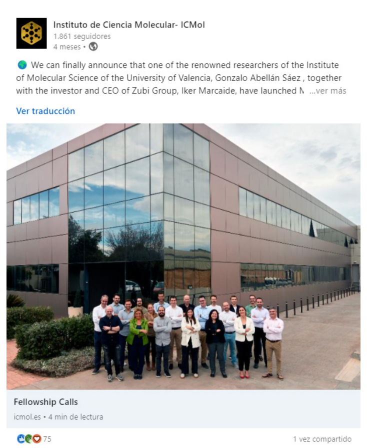


Social Media

Our presence on LinkedIn is focused on highlighting the significant achievements, innovations, and advancements emerging from our research and collaborations.

A crucial part of our strategy on LinkedIn involves the promotion and dissemination of news related to our startups or "spin-offs". These entities, born from the ingenuity and cutting-edge research within the Institute of Molecular Science (IMS), represent the direct application of our science to real-world needs, offering innovative solutions across various industrial sectors. By sharing their successes, technological advancements, and projects, we not only elevate the profile of these companies but also highlight the commercial potential of the research conducted at ICMol.

Furthermore, LinkedIn has proven to be an invaluable platform for spreading and highlighting our participation in science and technology fairs. These events are crucial for us, as they not only allow us to stay abreast of the latest development trends and advancements in the field but also provide a unique opportunity to interact with industry leaders, potential collaborators, and other researchers.



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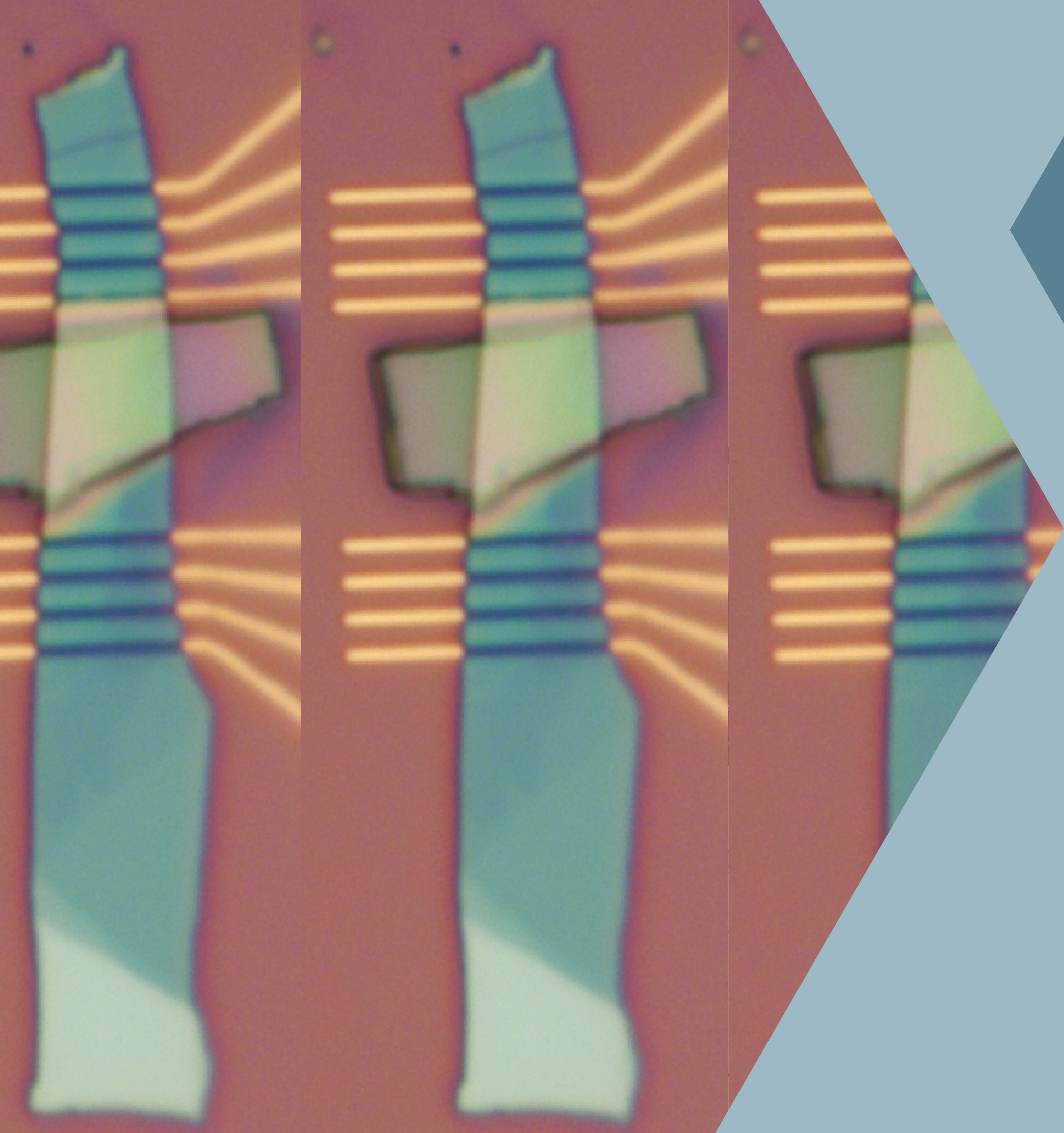

10

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2020

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