

DOCTORAL WORKSHOP

PhD in Chemistry

Scientific Programme and Book of Abstracts

May 22-23, 2025

Sala d'Actes

Faculty of Science

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**WELCOME TO THE XIII DOCTORAL WORKSHOP OF THE
PhD PROGRAMME IN CHEMISTRY**

May 22-23, 2025

It is our great pleasure to welcome you to the new Edition of the Doctoral Workshop of the PhD programme in Chemistry that is organized by the UAB's Department of Chemistry.

This year's workshop continues its tradition of providing supportive environment for doctoral students to present and discuss their dissertation with peers, members of the program and other experienced researchers, with the aim to strengthen the links and facilitating the exchange of research experiences and new ideas in the fields of entrepreneurship and small business.

During the event, 20 students, mostly on their third year will have an excellent opportunity to share their research. The Doctoral Workshop will also include an exciting series of plenary lectures given by international experts.

All the members of the PhD program in Chemistry and related programs, as well as other members of the research community are more than welcome.

We look forward to your participation in this event.

The Organizing Committee

ORGANIZING, SCIENTIFIC AND AWARDS COMMITTEE

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Dr. Xavier Sala, Coordinator and president of the academic committee of the PhD in Chemistry
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Dr. Daniel Maspoch, Vocal of the academic committee of the PhD in Chemistry
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INVITED SPEAKERS

Prof. Mircea Dincă
Princeton University



Mircea Dincă is the Alexander Stewart 1886 Professor of Chemistry at Princeton University. He grew up in Romania and moved to the United States to pursue his Bachelor's degree in Chemistry at Princeton University. Graduate studies in Inorganic Chemistry at UC Berkeley were followed by a postdoctoral appointment at MIT. He started his independent career in 2010 at MIT and moved his research group to Princeton in 2025. His group focuses on the synthesis of new multifunctional materials for applications in electrical and electronic devices, heterogeneous catalysis, and various uses in clean and renewable energy. In recognition of his group's research, Dincă has been awarded the Alan T. Waterman Award from the NSF in 2016, the ACS Award in Pure Chemistry in 2018, and the Blavatnik National Award in Chemistry in 2021, among several others. He has been named to the Thomson-Reuters/Clarivate Analytics Highly Cited Chemists List yearly since 2014.

Prof. Géraldine Masson
ICSN-CNRS/Paris-Saclay University



Géraldine Masson received her Ph.D. in organic chemistry from Joseph Fourier University (Grenoble, France) in 2003, under the supervision of Dr. Sandrine Py and Prof. Yannick Vallée. That same year, she joined the University of Amsterdam (Netherlands) as a Marie Curie postdoctoral fellow, working with Prof. Jan van Maarseveen and Prof. Henk Hiemstra.

In 2005, she became a CNRS researcher in the group of Prof. Jieping Zhu at the Institut de Chimie des Substances Naturelles (ICSN). She launched her independent research career in 2011 and has led the POWER group (Photocatalysis and Organocatalysis With Efficient Reactivity) since 2012. She was promoted to CNRS Research Director (DR2) in 2014 and to DR1 in 2020. In 2021, she became Co-Director of Labcom HitCat, a joint laboratory between SEQENS and the CNRS.

Her research focuses on the development of innovative catalytic methodologies for the synthesis of optically active, biologically relevant molecules, with particular emphasis on asymmetric organocatalysis and photoredox catalysis.

Prof. Charles Machan
University of Virginia



Charles Machan (muh-hahn) was born in Madison, WI and grew up in Wauwatosa, WI where he attended Marquette University High School before going to Washington University in St. Louis (WashU). While at WashU he played football for four years as a defensive tackle and majored in Chemistry and German (B.A. 2008). Charles attended Northwestern University for graduate school and completed a Ph.D. in Inorganic Chemistry (2012) under the supervision of Chad A. Mirkin. At Northwestern he served as President of the Alpha Gamma Chapter of Phi Lambda Upsilon, a co-ed chemistry honors fraternity, and received the Edmund W. Gelewitz Award for Outstanding Senior Graduate Student (2012). From 2013-2016 he was a postdoctoral researcher with Clifford P. Kubiak at the University of California, San Diego. Charles joined the Department of Chemistry at the University of Virginia in 2016 as an Assistant Professor. Since 2022, he has been an Associate Professor in the Department, where his research program currently receives funding from NSF and DOE. He received the Bessel Research Award from the Alexander von Humboldt Stiftung in 2024. His research covers energy-relevant catalysis involving abundant small molecules like carbon dioxide, dioxygen, dihydrogen, and water as reagents at the interface of molecular electrochemistry and materials. The approach focuses on developing new inorganic complexes and materials which incorporate co-catalytic moieties, non-covalent secondary sphere interactions, and substrate relays as catalysts to store electrical energy in chemical bonds.

SCIENTIFIC PROGRAM

May 22nd**08:45—09:00 Welcome and opening**

Prof. Lluís Escriche, Head of the Department of Chemistry

Prof. Rosa Maria Sebastian, Vicerector for Innovation, Transfer and Entrepreneurship

09:00—10:00 Plenary Lecture

Chair: Daniel Maspoch

Title: From electrically conductive MOFs to sustainable batteries**Prof. Mircea Dincă****10:00—10:45 Poster session + Coffee Break****10:45—12:00 Presentations I**

Chair: Maria Jesús Sánchez

- 10:45 - 11:00** Clip-Off chemistry as a synthetic tool towards unprecedented reticular and molecular materials. **Sara Ruiz Relaño**. P1.1
- 11:00 - 11:15** A Ni based OER photoanode working in CO₂RR conditions. **Aureliano Macili**. P1.2
- 11:15 - 11:30** Design of low-powered electrochromic devices using quasi-solid matrices on ionic liquids. **Tehreema Naeem**. P1.3
- 11:30 - 11:45** Light-induced HER using 2D-COF in multicomponent systems. **David Reyes Mesa**. P1.4
- 11:45 - 12:00** Atomistic modelling of corrosion inhibition: the role of oxides. **Mazhar Iqbal**. P1.5

12:00—13:00 Plenary Lecture (GEQO Seminarios Itinerantes)

Chair: Xavier Sala

Title: Metal-Free Molecules as Electrocatalysts and Co-electrocatalysts**Prof. Charles Machan****13:00—15:15 Break****15:15—17:15 Presentations II**

Chair: Xavier Solans

- 15:15 - 15:30** Sol-gel materials based on 1st row metals for water oxidation photoelectrodes. **Axel Guinart Guillem**. P2.1
- 15:30 - 15:45** Modelling Metals in Supramolecules – Proteins and Metallocages. **Mercè Alemany Chavarria**. P2.2
- 15:45 - 16:00** Process development towards Bismuth Subsalcylate. **Ruben Doblas Perez**. P2.3
- 16:00 - 16:15** Molecular modelling for the design of metal-containing biosystems: cytochrome P450 CYP199A4. **Laura Martínez Castro**. P2.4
- 16:15 - 16:30** Development of quantitative point-of-care devices for detection of infectious diseases. **Judit Prat Trunas**. P2.5
- 16:30 - 16:45** New azobenzene derivatives for selective light-modulated COX-2 inhibition. **Amanda Morales Jiménez**. P2.6
- 16:45 - 17:00** From Inflammation to Cancer: Computational modelling of key systems of interest. **Álex Pérez Sánchez**. P2.7
- 17:00 - 17:15** Polyethylene terephthalate microplastics staining with iDye Poly Pink: staining optimization and toxicity evaluation. **Uma Maheswari Mariappan**. P2.8

May 23rd

09:15—11:00 Presentations III

Chair: Rosario Núñez

- 09:15 - 09:30** Scalable Synthesis of Organic Molecules via Clip-off Chemistry from Covalent Organic Frameworks. **Juan Pablo Cavalieri**. P3.1
- 09:30 - 09:45** Inside-out functionalization of Rh(III)-Based MOPs. **Xiang Zhang**. P3.2
- 09:45 - 10:00** Absorption and reactivity in interstellar refractory materials: a quantum-mechanical study. **Niccolo Brancone**. P3.3
- 10:00 - 10:15** Synthesis of metal-organic nanosheets via clip-off chemistry. **Pilar Marina Fernández Serrián**. P3.4
- 10:15 - 10:30** Design of 2D Germanene nanoarchitectonics for implementation in energy and biosensing systems. **Yiming Lei**. P3.5
- 10:30 - 10:45** Synthesis of Spirooxazines with long lifetime of Merocyanine Form. **Mila Miroshnichenko**. P3.6
- 10:45 - 11:00** A novel nanotheranostic approach for glioblastoma based on nanocarriers and immune-PET radiopharmaceuticals (nanothera-PET). **Emily Betancourt Fernandez**. P3.7

11:00—12:00 Poster session + Coffee Break

12:00—13:00 Plenary Lecture

Chair: Carolina Gimbert

Title: Combined Asymmetric and Photoredox Catalysis for the Efficient Synthesis of Chiral Amines
Prof. Géraldine Masson

13:00—13:15 Award and Closing Ceremony

Doctoral Workshop 2024 distinguished Diploma, along with a gift, will be given to the two best Poster & Presentation.



Venue:

Plenary Lectures and PhD students' presentations: in the Auditorium of the Faculty of Sciences (*Sala d'Actes*).

Posters' Exhibition: in the Hall on the ground floor of the Faculty of Sciences (in front of *Sala de Graus I*).



ABSTRACTS

INVITED SPEAKERS

From electrically conductive MOFs to sustainable batteries

Mircea Dincă*

Department of Chemistry

Princeton University

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The emergence of electrically conductive metal-organic frameworks (c-MOFs) has been one of the most paradoxical developments in the field in the last few years. Indeed, how can one transport charges through a material that is mostly “empty” space? In this sense, MOFs made from layers of organic ligands connected by (typically) square-planar metal ions have shown particularly good electrical conductivity. However, a precise mechanism for charge transport is still the subject of debate, with various experimental and computational reports describing these materials as metals, semiconductors, or semimetals. This lecture will describe the latest efforts from our group to understand the intrinsic properties of 2D c-MOFs, especially as related to single-crystal electrical measurement studies, and will discuss in particular the unexpectedly large influence of out-of-plane transport. The seminar will also discuss how these fundamental studies have led directly to the discovery of a sustainable, organic cathode material that is competitive with incumbent oxides in Li-ion and Na-ion rechargeable batteries.

Combined Asymmetric and Photoredox Catalysis for the Efficient Synthesis of Chiral Amines

Géraldine Masson

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Nitrogen-activated carbon-carbon double bonds offer significant potential for constructing a diverse array of nitrogen-containing products. To expand the utility of these substrate

s, our research focused on investigating the reactivity of promising enamide derivatives.

We developed innovative methods for the α,β -difunctionalization of enamides using a synergistic two-step strategy that combines asymmetric organocatalysis with photoredox catalysis. A key aspect of this approach was the use of thiol as a transient reaction partner, which proved essential for enabling these transformations and synthesizing a diverse array of enantioenriched α,β -substituted amines.¹

Additionally, we successfully implemented stereoselective and enantioselective photocatalytic processes for synthesizing both α - and β -chiral amines. In these protocols, amino acids served as ideal linchpins, facilitating selective transformations and achieving high enantioselectivity.^{2, 3}

This lecture will highlight our contributions to these methodologies, with a particular focus on their applications in the synthesis of biologically active compounds.

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Metal-Free Molecules as Electrocatalysts and Co-electrocatalysts

Charles Machan

University of Virginia

There is continuously expanding interest in developing new electrocatalytic processes as an approach to harness intermittent electricity from renewable sources. Molecular systems are useful to understand and develop fundamental principles of these reactions through mechanistic study, as well as offer the possibility for testing structure-function relationships through iterative synthetic design. Broadly, the fundamental understanding of molecular species as electrocatalysts has relevance to the interconversion of electricity and chemical energy, as well as commodity chemical production. However, in order for homogeneous systems to eventually be scalable, their activity and stability must be improved. In naturally occurring enzymes, redox equivalents (electrons, often in a concerted manner with protons) are delivered to enzyme active sites by small molecules known as redox mediators (RMs). Inspired by this, we have been studying co-electrocatalytic systems which pair chromium-based homogeneous catalysts and metal-free RMs to convert carbon dioxide to carbon monoxide. The distinct advantage of the co-catalytic approach is the ability to independently select the properties of the secondary component without requiring catalyst modification. Based on these lessons from Cr-based co-electrocatalysis, we have more recently begun to examine the possibility of using metal-free molecules as electrocatalysts for the reduction of dioxygen. Interestingly, cationic conjugated organic molecules demonstrate catalytic activity for dioxygen reduction which has mechanistic parallels with well-studied Cu-based systems. Our results suggest that many new opportunities exist for refining reaction design for electrochemical transformations by systemically pairing redox-active small molecules with catalytic active sites, as well as imply that comparable design principles to transition metal-based electrocatalysts can be used develop and optimize organic-based ones.



ABSTRACTS

PhD STUDENTS

(In order of presentation)

Clip-off Chemistry as a synthetic tool towards unprecedented reticular and molecular materials

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Keywords: reticular materials, bond cleavage, metal-organic complexes

New molecules and materials are and will continue to be pivotal to our society; consequently, their design and synthesis will remain a vibrant challenge for chemists. While the focus of chemical processes has historically been on bond formation, the emergence of bond cleavage to achieve similar purposes is a notable development.

In this context, our group has introduced the concept of Clip-off Chemistry, a novel synthetic approach that generates new molecules and materials through the selective and rational covalent bond cleavage in reticular materials.^{1,2} Reticular materials are a class of chemical structures generated by connecting molecular building blocks (*e.g.* metal nodes and organic linkers) into crystalline, porous and extended solids as Metal-organic Frameworks (MOFs), or Metal-organic Polyhedra (MOPs).³ During the assembly of its initial components, repetitive subunits and fragments are spontaneously formed within the final network, including clusters, macrocycles, cages, and chains. These fragments represent a new source of molecules and materials when they are selectively isolated from the reticular precursors.

In this study, we select MOFs and MOPs as reticular precursors to synthesize new metal-organic complexes such as clusters and cages, among others. We demonstrate that the insertion of cleavable bonds (*e.g.* olefinic bonds) in suitable positions within Rh(II)-based MOP precursors, followed by a selective bond cleavage reaction (*e.g.* ozonolysis), leads to the synthesis of four new aldehyde-functionalized Rh(II)-based complexes, including a homoleptic cluster, *cis*-disubstituted cluster, a macrocycle, and a crown.⁴ Furthermore, the synthetic approach is validated by incorporating olefinic bonds within a three-dimensional *rht* Cu(II)-based MOF and subsequently cleaving the precursor into its constituent fragments, yielding novel multivariate and aldehyde-functionalized cuboctahedra Cu(II)-MOPs (Figure 1).⁵

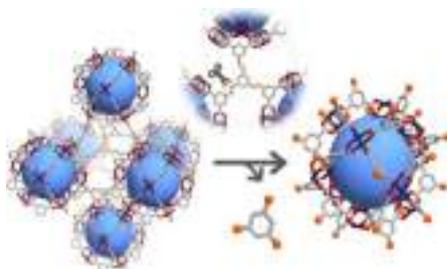


Figure 1. Clip-off Chemistry approach to obtain Cu(II)-MOPs from the selective bond cleavage

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A Ni based OER photoanode working in CO₂RR conditions

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Laia Francàs¹, Jordi García-Antón¹, Xavier Sala¹

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The electrochemical conversion of solar power into energy vectors is a crucial component of the future decarbonization of societies. This catalytic process allows the storage of renewably obtained energy into chemical bonds of vector molecules. Carbon-based fuels and chemicals can be sustainably synthesized by electrochemically reducing carbon dioxide (CO₂RR) at a cell's cathode. In aqueous electrolytes, the CO₂RR reactions are often coupled to the Oxygen Evolution Reaction (OER) at the anode. While Ni-based catalysts are the benchmark for OER in alkaline electrolysis [1,2,3], their performance declines in the neutral and carbonate-rich conditions which are typical of CO₂RR [4]. SOREC₂, is an EU-funded initiative [5] which aims to develop technologies to convert solar photons and CO₂ into species containing C-C bonds like ethanol or ethylene (C₂ products). The project is based on the development of a compact tandem Photoelectrochemical Cell (PEC) featuring an engineered cathode, designed to enhance selectivity toward C₂ products.

This presentation will focus on the synthesis and characterization of a novel Ni-based OER catalyst, and its incorporation in photoanodes capable of operating under the restrictive conditions of CO₂RR. The material is fabricated via an organometallic approach [6], using a bifunctional ligand, this yields a nanocatalyst embedded in a protective matrix that enhances stability at pH 7 and in carbonate environments. Additionally, this unique nanostructure allows the grafting of the catalyst to oxide-based semiconductors, enabling the fabrication of stable, transparent photoanodes essential for assembling the CO₂RR-OER PEC.

Extensive characterization of the catalyst and photoanodes has been conducted through various techniques, including *operando* XAS and high-resolution HAADF-STEM mapping, in collaboration with the ALBA synchrotron.

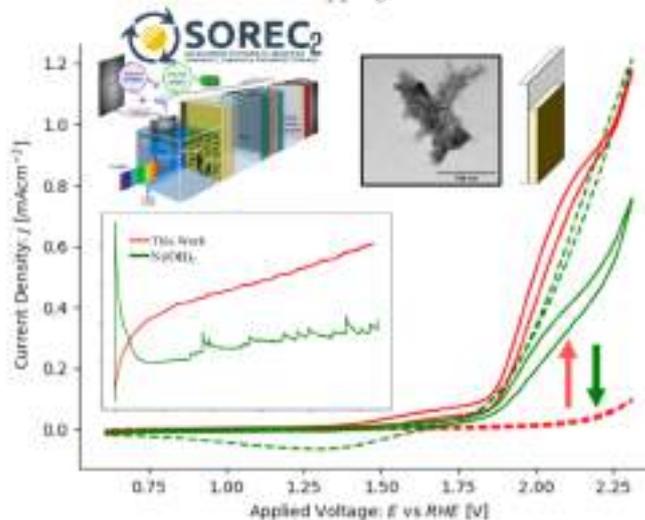


Figure 1. SOREC₂ stack, TEM image of the catalyst and electrochemical measurements.

Keywords: CO₂RR, OER, Photoelectrochemistry, Nanocatalyst

References:

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Design of low-powered electrochromic devices using quasi-solid matrices based on ionic liquids

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Ionic liquids (ILs) and ionogel (IG) membranes are innovative components within the realm of functional electrochemical materials, demonstrating outstanding tunability, thermal stability, electrochemical performance, and environmental friendliness [1]. A rising trend is to fabricate ionic liquid electrolytes into solid electrolytes to address the risk of leakage due to their liquid nature. This study investigates the integration of ILs into solid-state ionogels, creating hybrid systems that effectively combine the benefits of liquid electrolytes with solid-state devices. Hence, this presentation underscores the relationship between IL chemistry and ionogel architecture, paving the way for innovative smart material designs to advance energy-efficient display technologies and beyond.

For ionogel preparation, we selected poly(vinylidene fluoride-*co*-hexafluoropropylene) (PVDF-*co*-HFP)-as a solid polymer matrix, and we used *p*-nitrobenzyl bromide (*p*-NBBBr) as a model redox compound to optimize the fabrication method, mechanical properties and ionic conductivity of IGs [2]. After that, we tackled their application for building solid-state electrochromic devices (ECDs). In our case, dimethyl terephthalate (DMT) was selected as the electrochrome due to its electro-optical properties [3]. Cyclic voltammetry and in-situ spectroelectrochemistry techniques were used to investigate the electrochromic mechanism and properties of the DMT@IG system. The DMT-based ECD exhibits high stability and low operating voltage, presenting bleaching and coloring times of 7.89 and 4.71 seconds, respectively, with 63.6% optical contrast (ΔT) and a good color efficiency (CE) of 147.7 cm²/C, with device stability of up to 30 cycles. Finally, three-electrode and two-electrode displays were also fabricated with a DMT@IG membrane to demonstrate the potential of using DMT-based displays for electrochromic devices.

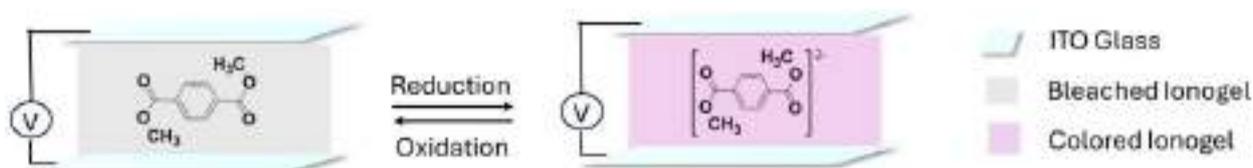


Figure 2: Graphical representation of the DMT@IG system in 2-electrode setup exhibiting electrochromic behaviour.

Keywords: Electrochemistry, Ionic liquids, Ionogel membranes, Electrochromic devices

References

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Light-induced HER by using 2D-COF in multicomponent systems

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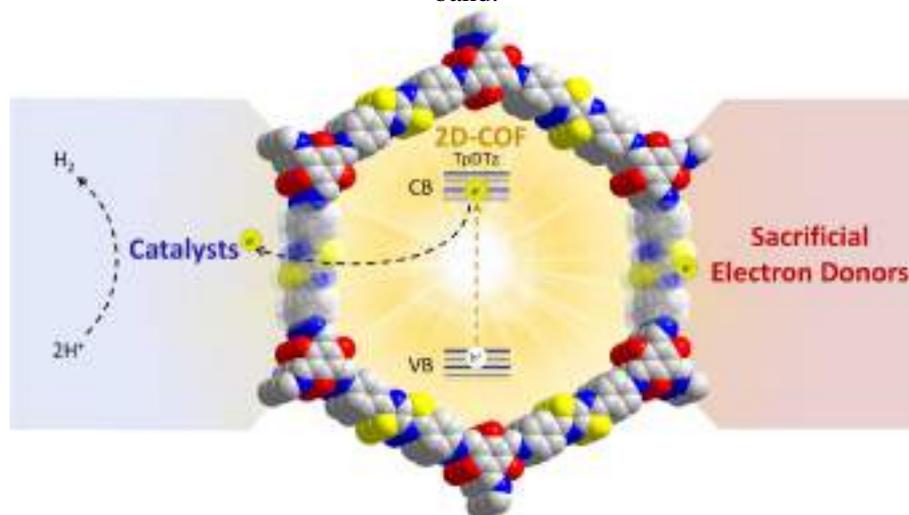
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Due to the current worldwide situation, the use of green fuels is on the rise, with green hydrogen emerging as one of the most promising options. Generation of hydrogen through water splitting under visible-light irradiation has been a known topic for a long time now.^{[1],[2]} Photochemical water splitting is a complex process in which different components are required to fulfill the overall reaction, each of them having a key role including (i) harvesting the light, (ii) separation of charges, (iii) breaking and (iv) formation of chemical bonds.

Organic semiconductors have recently emerged as promising materials to be used in photocatalysis. Prominent examples of this family of semiconductors are 2D-covalent organic frameworks (COFs), which are reticular materials with high crystallinity and porosity.^[3] They have been applied to photocatalysis including visible light-induced hydrogen evolution reactions (HER) with great success.^{[4],[5]} One of the advantages of COF materials is their versatility to control chemical and electronic structure, allowing to rationally design better photocatalytic materials by enhancing solar light harvesting, charge separation, interaction with catalytic species or dispersibility in water.^[6]

In this work we have prepared a family of 2D-COF materials by adding different moieties to the organic skeleton and tested the material for light-induced HER in combination with well-defined catalytic centers and suitable electron donors (Chart 1).

Chart 1. Schematic representation of the multicomponent system. VB: valence band. CB: conduction band.



Keywords: Covalent Organic Framework (COF), green hydrogen, visible light, photocatalysis.

References

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Atomistic modeling of corrosion inhibition: the role of oxides

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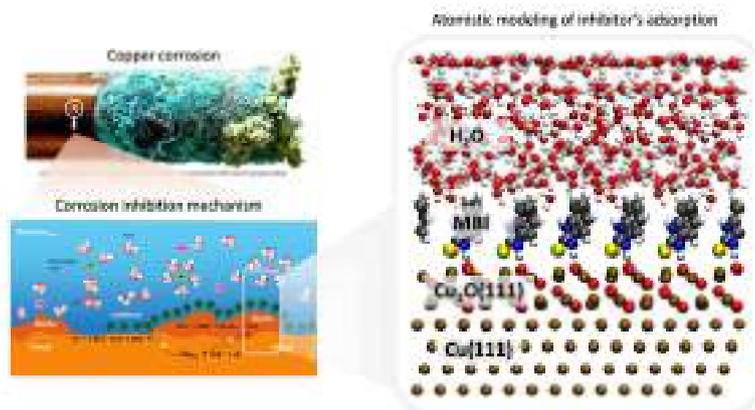
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In an open atmosphere, the degradation of metal (corrosion) is due to several electrochemical reactions of metal surfaces with atmospheric corrosive species such as oxygen, moisture, and electrolyte ions. An efficient and cost-effective way for corrosion prevention is the application of small organic molecules (corrosion inhibitors) on metal surfaces which provide shielding from atmospheric corrosive species by creating an effective film barrier. An atomistic understanding of chemistry at the inhibitor-metal interface is significant in the design of novel inhibitors. Molecular modeling stands as an excellent tool compared to time-consuming and expensive experimental techniques in this regard¹. Our research group is working to improve the available modeling approaches, aiming to develop a computational methodology that can describe inhibitor orientation and interactions at the inhibitor-metal interface and the effect of corrosive media on inhibitor binding.

We are examining 2-mercaptobenzimidazole (MBI) since it is experimentally well-known to be an efficient corrosion inhibitor for copper (Cu). The objective of the current modeling study is to evaluate how aqueous solution and corrosive potential influence MBI adsorption and the charge redistribution at the inhibitor/oxidized Cu interface. We address this problem by employing density functional theory (DFT) as implemented in the SIESTA code. Our findings revealed some stable orientations of MBI molecules at low and high coverages on oxidized Cu surfaces, which were not reported in the literature. In addition to that, we performed ab initio molecular dynamics to fully incorporate the solvent effects, and our results show that solvent molecules stabilize the MBI@N-H bond that keeps breaking and forming during simulations performed in a vacuum. We are confident that our approach can pave the way to investigate the corrosion of materials, representing an important progress for the area.

Figure:



Keywords: Copper corrosion inhibition, copper oxide-water interface, DFT, AIMD

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Sol-gel materials based on 1st row metals for water oxidation photoelectrodes

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The production of benign fuels from clean and renewable source of energy is a stimulating goal.¹ In this context, the scientific community draws inspiration from nature to design artificial photosynthetic systems.² Artificial photosynthesis aims to achieve the light-induced water splitting ($2\text{H}_2\text{O} \rightarrow \text{O}_2 + 2\text{H}_2$), that consists in the hydrogen evolution reaction, HER ($4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2$), for which protons and electrons are supplied by the water oxidation reaction, WOR ($2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 4\text{e}^-$). Since WOR is thermodynamically and kinetically demanding, it requires efficient water oxidation catalysts (WOCs) to overcome its activation barrier.³ The best WOCs reported today are made of Ru and Ir. However, it is highly desirable to use more Earth-abundant transition metals, whether in the form of metal complexes (MC) or metal-oxide nanoparticles (MO-NPs).⁴

In this project, we design an anodic catalytic layer to be incorporated in a water splitting electrochemical cell based on a hybrid thin film of SiO_2 containing WOC units based on first-row transition metal catalysts, whether in form of MO-NPs or MCs. This approach aims to achieve i) protection against degradation, and ii) the attachment of an active WOC capable of sustain operational current at low overpotentials, ensuring iii) high conductivity. We present two candidates to achieve optimal performance activity, a cobalt oxide NPs and a MC based on a Cu macrocyclic unit (Cu-MAC) known to be an efficient WOC at different values of pH.⁵ Both candidates will be incorporated into stabilizing SiO_2 matrixes (Figure 1).

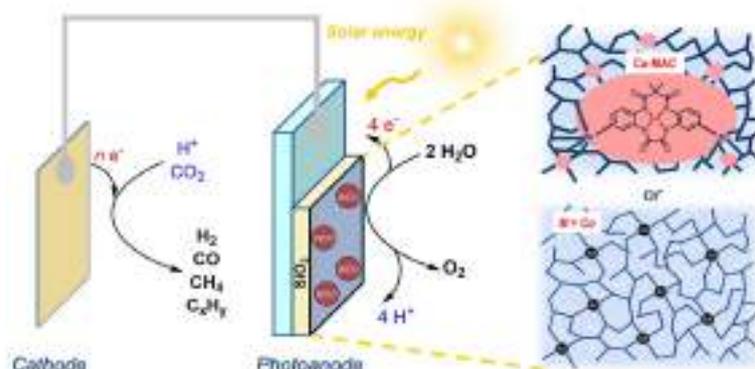


Figure 3: Schematic water splitting photoelectrochemical cell based on a photoanodic hybrid SiO_2 deposit

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Keywords: Water oxidation catalyst, hybrid silica material, first-row metal catalyst, photoanode, energy conversion.

Modeling Metals in Supramolecules - Proteins and Metallocages

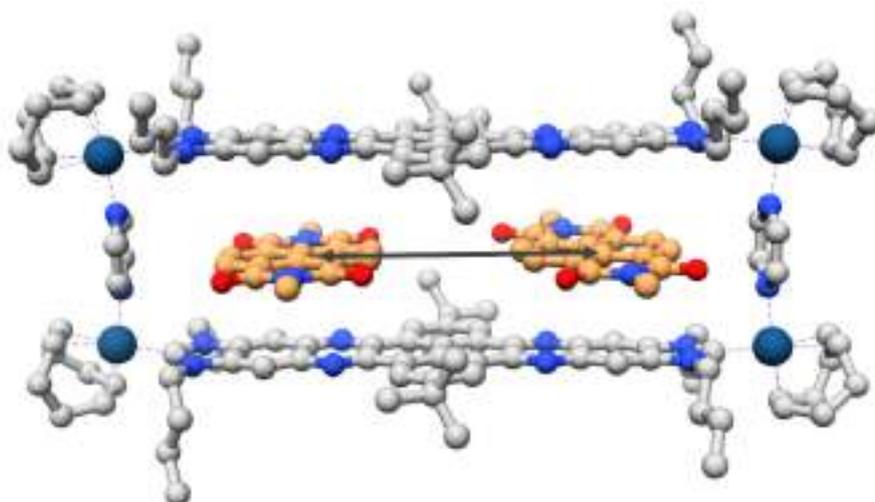
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Metals have an important role in life; about 30% of proteins contain metal atoms either for structural or catalytic purposes. Metals have also an important role in the rising field of supramolecular chemistry, allowing a wide range of geometries and functionalization for self-assembled metallocages [1].

Modeling how metals behave within organic systems is a challenge because of their inherent complexity. The present work employs a set of computational techniques applied to systems whose architectures stand on metal interacting with synthetic and natural ligands. This includes cytochrome P450 model interacting with inhibitors with pesticide potential [2], and the mechanisms through which a guest is encapsulated into a metallocage [3-4].

All these works also stand on multi-scale strategies where different methodologies are combined to reach clear insights on the systems of study. These techniques range from Molecular Docking, Molecular Dynamics, and enhanced sampling methods like Metadynamics and Gaussian accelerated Molecular Dynamics.



Keywords: Protein structure, Metallocages, Structural Recognition, Metadynamics, Molecular Dynamics

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Process development towards Bismuth Subsaliolate

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A novel synthetic process to produce bismuth subsaliolate, a widely used pharmaceutical active ingredient based on a bismuth salt, has been developed to overcome key limitations of the traditional method used in OCB Pharmaceutical. The previous process involved multiple steps, utilized bismuth subnitrate as an intermediate, and offered limited control over quality modulation (physical properties). The new process enables a one-step synthesis directly from bismuth nitrate solution, with enhanced capacity to modulate product quality.

The process development was initially studied at laboratory scale by exploring the influence of reaction parameters. These tests led to successful synthesis of BSS meeting quality specifications. However, preliminary scale-up batches exhibited non-conformities due to the presence of critical impurities, prompting a comprehensive root cause analysis. Two major impurities were identified: soluble bismuth, linked to incomplete conversion of bismuth subnitrate, and a coloured impurity attributed to nitrosaliolate acid formation. These hypotheses were experimentally validated through targeted laboratory studies and confirmed using advanced analytical techniques, including X-ray diffraction and HPLC-MS. Two statistically designed experiments (DoEs) were conducted to define optimal process conditions, ensuring consistent formation of the reactive bismuth species and suppressing impurity generation. The final process was developed under a Quality by Design (QbD) framework and supported by risk-based assessments, resulting in a robust, scalable, and reproducible synthesis. This development represents a significant advancement in the manufacturing of bismuth subsaliolate, improving efficiency, quality control, and industrial applicability.

Keywords: Bismuth Subsaliolate, Process Development, Impurity control, Quality by Design, One-step Synthesis.

Molecular Modelling for the design of metal-containing biosystems: cytochrome P450 CYP199A4

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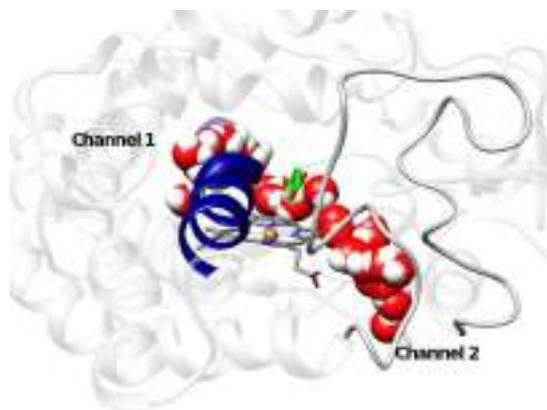
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Metals are involved in up to 40% of proteins archived in the Protein Data Bank. They are not only essential for the proper functioning of living organisms but also show exceptional characteristics for their application in different fields like industry or biomedicine. One of the largest metal-containing families of proteins are cytochromes P450. These hemoenzymes are responsible for the catalysis of oxidative reactions across all kingdoms of life, and they have been widely studied for their role in drug metabolism but also as the basis for biocatalyst design. [1]

In collaboration with Dr. S. Bell's group in Australia, we have studied CYP199A4, a cytochrome P450 from the bacterium *Rhodopseudomonas palustris*. This highly versatile organism has developed the ability to catalyse a wide variety of reactions involving benzoic acid derivatives. [2]

To complement the available experimental data, including crystallographic structures of both substrate and product-bound states, we conducted a computational study aimed at elucidating key aspects of the catalytic process. Specifically, we examined the source of specificity in CYP199A4, potential pathways for substrates and products to the active site, and the role of solvation in the mechanism. The primary computational approach employed was Gaussian accelerated Molecular Dynamics (GaMD), supported by extensive bioinformatic analysis. [3]



Keywords: Molecular modelling, enzyme design, metalloenzyme, molecular dynamics, cytochrome P450.

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Development of quantitative point-of-care devices for detection of infectious diseases

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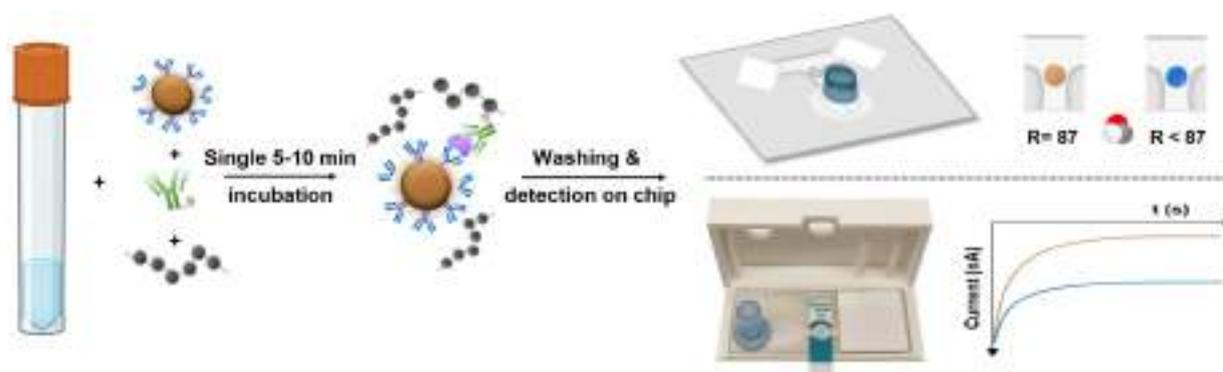
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Biosensors are bioanalytical devices that incorporate a molecular recognition element (bioreceptor) associated to, or integrated with, a physicochemical transducer. In this way, analyte biocapture is directly translated into a measurable signal. To date, numerous biosensors have been developed using a wide variety of biorecognition elements and transducers to maximize their cost effectiveness, rapidity, portability and robustness when compared to more complex and classical analytical tools. Among them, electrochemical immunosensors are relatively cost-efficient, specific and easy to miniaturize, which coupled to integrated microfluidics allows developing point-of-care testing (POCT) devices to be used directly by the patient or at the surgery. Nevertheless, classical immunosensors display a few limitations too. For example, electrode modification (such as for antibody incorporation) produces its partial blocking, which has a negative effect on electron transfer compared to bare electrodes. For this, magneto-immunoassays (MB-assays), working with magnetic beads to capture the analyte and concentrate it onto the electrode, have been shown to grant faster analyte binding, higher maximal signals and lower limits of detection than classical two-dimensional immunosensors. Nevertheless, MB-assays entail tedious MB handling, which is not compatible with POCT. In this thesis project paper-based devices have been produced to achieve partial-automation of MB-assays with simple microfluidics. The detection of different infectious diseases, including malaria and respiratory viral infections, has been achieved, providing sensitive and quantitative results in less than 20 and 40 min for the electrochemical and colorimetric readouts, respectively. The project has focused on improving the performance of such devices evaluating different types of micro/nanomagnetic beads, paper-based materials and device geometries, and transduction strategies. The final goal is to validate those devices in the field to ensure their performance outside an equipped laboratory.

Keywords: Point of care testing (POCT), infectious diseases, magnetic beads, paper-based immunoassays, automation.



New azobenzene derivatives for selective light-modulated COX-2 inhibition

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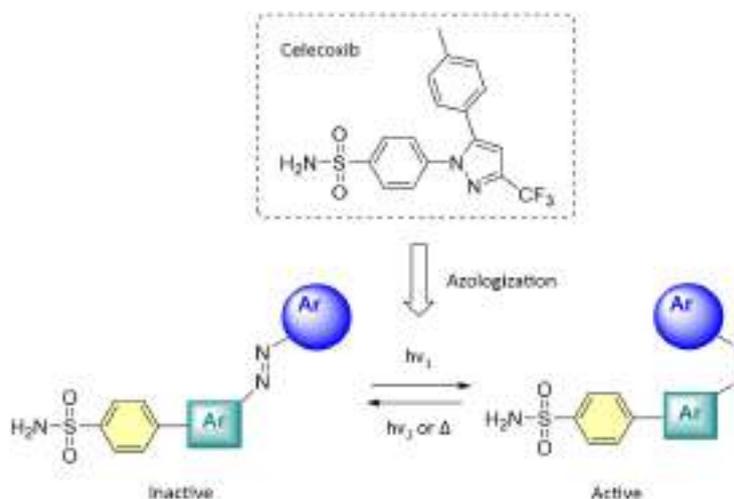
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The enzyme cyclooxygenase COX-2 is transiently expressed during inflammatory processes and is usually associated with some of the main symptoms derived.¹ As a result, it is the principal therapeutic target of non-steroidal anti-inflammatory drugs (NSAIDs) such as acetylsalicylic acid and diclofenac, which act as pain and fever killers by inhibiting COX-2 activity.² However, NSAIDs are nonselective and they also actuate on constitutive COX-2 and COX-1 enzymes found in normal tissues, which regulate some relevant physiological functions. Consequently, these drugs lead to a plethora of side effects such as ulcers or kidney problems.² To overcome these drawbacks, it is therefore required to develop COX-2 inhibitors whose therapeutic activity can be confined to the inflamed tissues. By producing light-sensitive drugs that can be reversibly activated with spatial and time control, photopharmacology offers great promise to accomplish this objective.³

To pioneer the development of photopharmacology tools for light-controlled COX-2 inhibition, we are focusing our attention on Celecoxib, an approved selective COX-2 inhibitor which however is associated with increased cardiovascular risk. To make the therapeutic activity of this compound photoswitchable, we are employing an azologization strategy based on computational studies. We have designed Celecoxib derivatives incorporating a photoisomerizable azoaromatic group and evaluate the differential interaction of their *trans* and *cis* isomers with the binding site of COX-2 using molecular dynamics. As illustrated in the figure, the target derivatives must remain inactive in the *trans* form, while selectively interact with COX-2 upon photoconversion to their *cis* state. Then, the most promising candidates identified in our calculations are synthesized and characterized photochemically. Finally, their COX-2 inhibition activity is evaluated by means of *in vitro* enzymatic studies. In this presentation we will discuss the best of the photoswitchable Celecoxib derivatives developed to date, with which we have already accomplished light-modulated COX-2 inhibition.



Keywords: COX-2, Coxib, Celecoxib, Photoswitchable ligand, Azobenzene compound.

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From Inflammation to Cancer: Computational Modelling of Key Systems of Interest

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Keywords: chronic inflammation, GPCRs, molecular dynamics, lipid mediators, maresin-1

Chronic inflammation is widely known to be the responsible for the development and progression of cancer. Our recent computational research tries to find out how inflammation and cancer are related at the molecular level, and how this could improve therapies. Our main players are cyclooxygenase (COX-2), leucine-rich G protein-coupled receptor type 6 and EP4 receptor.

COX-2 helps produce molecules that promote inflammation, is found at high levels in many cancers, and is known to support tumour growth. We have studied in detail how COX-2 works and the link of the dimer of the enzyme with cancer cells.¹ We are focused on developing new types of inhibitors that can be controlled with light or that target the dimer of COX-2. These new strategies could reduce side effects compared to traditional anti-inflammatory drugs. We also studied the pro-inflammatory receptor EP4, which is activated by prostaglandin E₂ (PGE₂). EP4 is known to play a role in cancer by increasing tumour growth, spreading, and blocking immune responses.² We have studied how EP4 is activated and how it interacts with G proteins involved in the signalling of that type of processes.

Our research also analyses how the human body resolves inflammation. We've studied a molecule called maresin-1, which naturally helps reduce inflammation and repair tissue. It works by activating the LGR6 receptor.³ We have studied the molecular behaviour of this compound and other lipid mediators to understand how they affect the mechanism of activation of the pro-resolution LGR6 receptor.

Altogether, these studies show how computational methods can give us an understanding for the complex links between inflammation and cancer. This approach helps explain how cancer develops and opens the door to designing new targeted treatments that could improve inflammation-based therapies..

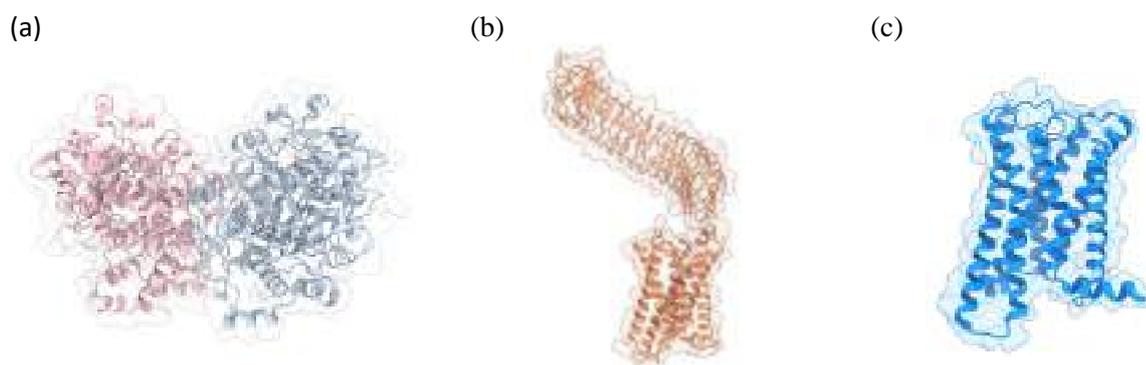


Figure 1. Structural 3D representation of (a) COX-2, (b) LGR6 receptor and (c) EP4 receptor.

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Polyethylene terephthalate microplastics staining with iDye Poly Pink: staining optimization and toxicity evaluation

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Labelling microplastics (MPLs) facilitates monitoring them in complex environmental and biological matrices. From previous studies¹, iDye Poly Pink (iDPP) was found to be the dye exhibiting the most advantages in MPLs monitoring, but this may introduce toxicity to biological systems, including microbial cells and intracellular environments. This study optimizes the staining protocol to minimize biological interference and evaluates the toxicity of the iDPP-stained polyethylene terephthalate (PET) MPLs. To do so, a design of experiments (DoE) was prepared, evaluating the interaction of three factors: the staining temperature, the PET MPLs concentration, and the iDPP dye concentration (Fig. 1a). Finally, with the optimal conditions, respirometry with potassium ferricyanide was conducted to assess the toxicity of iDPP-stained PET MPLs on the metabolism of *Escherichia coli* (Fig. 1b). Toxicity assessment revealed that iDPP-stained PET MPLs did not interfere with bacterial metabolism, indicating their suitability for non-disruptive labelling of PET MPLs for environmental and biological studies.

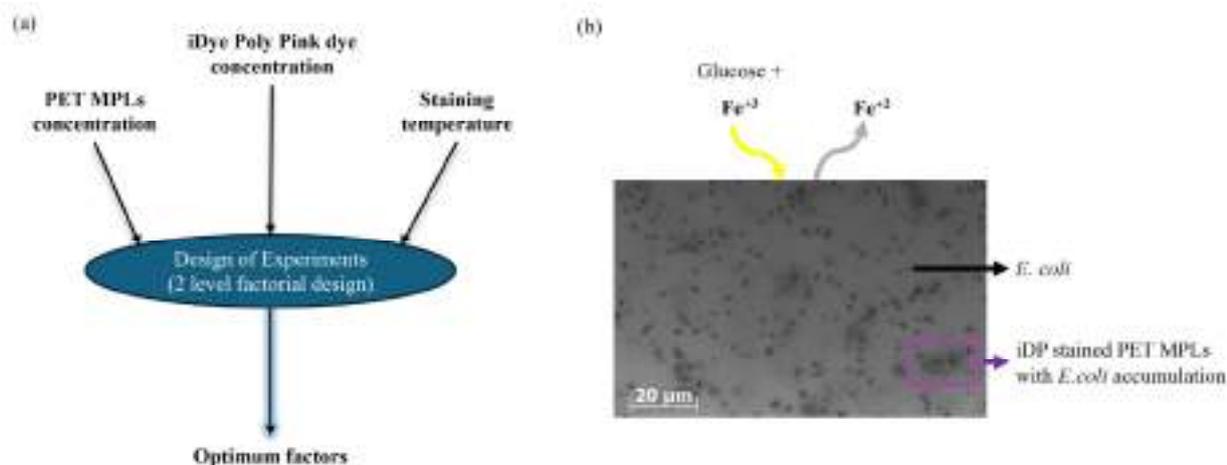


Figure 1: (a) Design of Experiments for the optimization of polyethylene terephthalate microplastics staining with iDye Poly Pink, (b) Fluorescence microscopy image of *E. coli* (syto 9) treated with iDye Poly Pink stained polyethylene terephthalate microplastics (Mag. 40X).

Keywords: iDye Poly Pink staining, polyethylene terephthalate microplastics, potassium ferricyanide respirometry, staining optimization, toxicity evaluation.

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Scalable Synthesis of Organic Molecules via Clip-off Chemistry from Covalent Organic Frameworks

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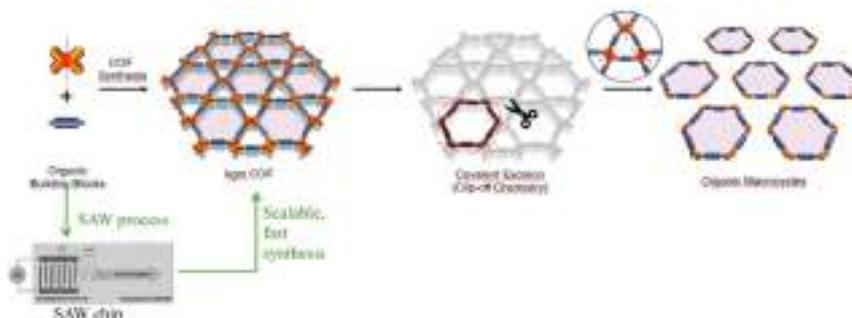
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Synthetic organic chemistry has long centered on designing and constructing new molecules for societal benefit, driven by the development of innovative synthetic methodologies and reactions that challenge conventional approaches to molecular assembly. Traditionally, small organic molecules can be synthesized via stepwise reactions involving simpler precursors.^[1] However, these strategies often fall short when applied to the efficient construction of structurally complex materials with high degrees of freedom, such as organic macrocycles, cages, catenanes, or intricate polymers.

In this work, we introduce a paradigm shift in the synthesis of functional organic molecules through a strategy we term *Clip-off Chemistry*.^[2-4] This approach enables the selective excision of target molecules from highly ordered, extended organic architectures—specifically, covalent organic frameworks (COFs). COFs are crystalline, two- or three-dimensional materials that not only embody their constituent building blocks but also serve as precursors for more complex structures like macrocycles, cages, catenanes, or polymers, which form spontaneously during their construction. By breaking specific bonds at predetermined sites within the framework, these complex molecular architectures can be released with remarkable selectivity and yield.

We demonstrate the effectiveness of this Clip-off Chemistry strategy for the synthesis of functional organic macrocycles, overcoming traditional obstacles such as poor selectivity, low yields, unwanted side products, and labor-intensive purification. Clip-off Chemistry allows for the gram-scale, selective synthesis of macrocycles—structures that typically require precise control to prevent the formation of linear oligomers or smaller rings. In this work, we report the successful synthesis of nine hexagonal macrocycles with polyamide and polyimide linkages, featuring peripheral aldehyde and carboxylic acid groups. Furthermore, we show that this method can be integrated with isorecticular chemistry to precisely tune macrocycle size and functionality. This enables access to increasingly large macrocycles, including 114-, 138-, and 162-atom rings, and allows for the incorporation of functional groups such as fluorine.

Despite the possibility to scale-up our clip-off of COFs process, the scalability of the COF precursor remains a bottle-neck for the industrial exploitation of our methodology. To address this, we explored the use of surface-acoustic waves (SAWs) as a mild method for the rapid synthesis of large quantities of COF.^[5] The technique allows the simultaneous synthesis and coating of COFs at room temperature onto a variety of substrates, enhancing not only the industrial preparation of COF precursor but also their processability.



Scheme 1. Schematic representation of clip-off of COF approach and how SAWs are used in the process.

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Keywords: clip-off chemistry, covalent organic frameworks, macrocycles, ozonolysis, surface acoustic waves.

Inside-Out Functionalization of Rh(II)-Based MOPs

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Keywords: *Metal-Organic Polyhedra (MOPs), cages, Internal functionality, Outside functionality*

Metal–organic polyhedra (MOPs) are porous coordination cages constructed from metal ions and organic linkers. Robust MOPs, particularly those based on Rh(II) nodes, exhibit distinctive features such as nanometric dimensions (typically 2–5 nm) and molecular-level reactivity, which can be explored under homogeneous conditions using spectroscopic and crystallographic techniques. These attributes place MOPs at the interface of molecular and nanoscale chemistry, motivating their designation as “molecular nanoparticles.”

In this seminar, we present recent advances in broadening the chemical functionality of MOPs. We report new surface modifications incorporating phosphate and dihydroxy groups, as well as internal functionalization with amine groups (Figure 1). The MOPs described here are novel and represent previously unreported architectures. These functionalities enable new directions in host–guest chemistry—particularly with endohedrally amine-functionalized MOPs—and hierarchical self-assembly using surface-functionalized analogues. Altogether, these developments underscore the potential of MOPs as versatile molecular platforms for the design of next-generation functional materials.

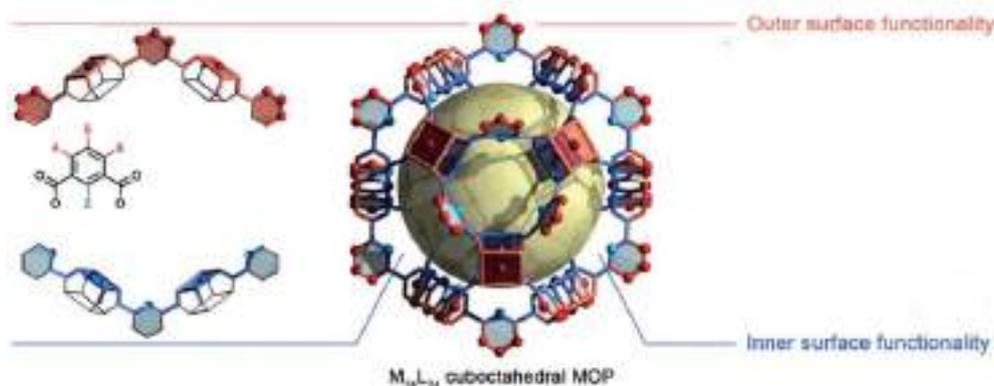


Figure 4. The reaction of the internal and external reactive sites with $M_{24}L_{24}$ Cuboctahedral MOP.

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Adsorption and reactivity in interstellar refractory materials: a Quantum-mechanical study

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This study explores different challenges related to astro- and prebiotic chemistry in rocky astronomical bodies—comets, asteroids, planetesimals, and exoplanets—using Density Functional Theory (DFT) methodologies. A first part of the work focuses on the modelling of the surface-mediated prebiotic self-oligomerization of hydrogen cyanide (HCN), a highly reactive molecule known to oligomerize into adenine under basic conditions or on ionic surfaces [1, 2]. Accordingly, each step of the HCN tetramerization into diaminoacetonitrile (DAMN, $H_4C_4N_4$)—a key intermediate in adenine synthesis—was investigated when catalyzed by crystalline Mg_2SiO_4 (forsterite), the most prevalent mineral in rocky astronomical bodies. The study began with a DFT-based characterization of the structural and energetic features of various periodic forsterite surfaces, followed by an in-depth analysis of HCN adsorption behavior on them. Multiple dimerization pathways of HCN to iminoacetonitrile (IAN, $H_2C_2N_2$) on these surfaces were examined, and their Potential Energy Surfaces (PESs) were computed in detail. The most favorable dimerization case was then extended to complete DAMN formation. While the HCN oligomerization is hindered in the gas phase [3], forsterite proves to be an effective natural catalyst for the reaction due to the occurrence of both Lewis acidic and basic sites on its surfaces [4], allowing for: *i*) an effective activation of the molecule via deprotonation, *ii*) facilitated C—C bonds formations, helping the growth of the oligomeric backbone, and *iii*) the exothermic formation of DAMN. Still, a further catalytic effect by water is necessary to help the very last steps of the reaction. Notably, relatively stable forsterite surfaces show greater catalytic efficiency than less stable ones, offering an optimal balance between the activation of HCN (via deprotonation) and, thanks to not too strong adsorptions, sufficient surface mobility to permit reaction. RRKM kinetic analyses indicate that HCN oligomerization to DAMN is favored at temperatures typical of more evolved bodies (~300 K), while it is hindered below 150 K—consistent with both observations and experimental data. [2, 5]

The work also presents *ab initio* spectral simulations for systems of prebiotic interest to support the interpretation of experimental results. A combined theoretical–experimental study was carried out on the electronic Circular Dichroism (CD) and anisotropy (*g*) spectra of the chiral molecules glycidol and butanediol, within the framework of the hypothesis that homochirality in sugars and amino acids in the Solar System originated from irradiation by natural Circularly Polarized Light (CPL). [6] The CD and *g* spectra, measured in the vacuum ultraviolet (VUV) region, were successfully reproduced using Time-Dependent DFT (TD-DFT), allowing for the identification of molecular orbitals (MOs) involved in the low-energy electronic transitions, explanation of shifts due to water solvation, and assessment of the method's strengths and limitations in this context. Infrared (IR) spectra of HCN–forsterite systems at low temperatures ($T < 150$ K, under non-reactive conditions) were also simulated and compared with experimental data. Owing to the high number of degrees of freedom in these systems, a nonlinear, non-energy-weighted best-fit procedure between computed and experimental spectra was employed, allowing for the accurate identification of molecular species and the dominant forsterite surfaces involved. This second section emphasizes the crucial role of theoretical simulations in the interpretation of experimental spectroscopic results and outlines various strategies for modeling spectra of systems with differing complexities and measurement techniques.

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Synthesis of Metal-Organic Nanosheets via Clip-Off Chemistry

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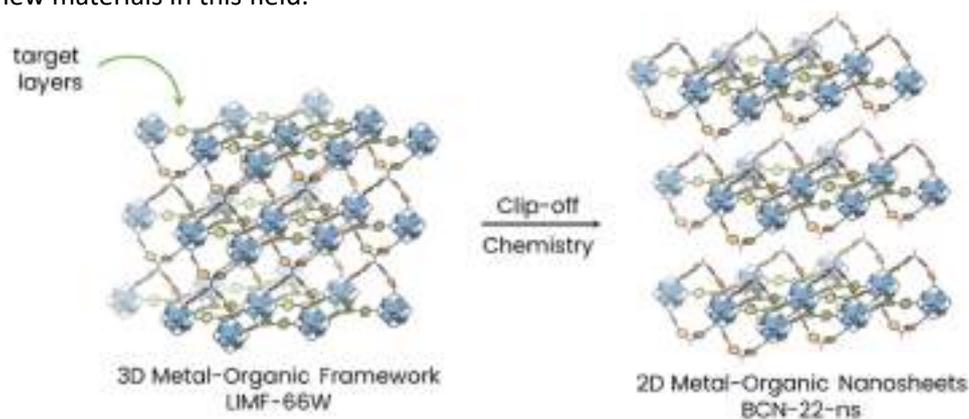
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Two-dimensional (2D) nanomaterials have gathered great attention in the field of Materials Science due to their high surface to volume ratio, which results in excellent physical and chemical properties valuable in different fields such as catalysis, energy storage or separation [1]. In this regard, Metal-Organic Frameworks (MOFs), which consist of highly crystalline architectures of periodically connected inorganic metal-based nodes through organic linkers, offer a significant advantage because of their superior ease of design. The obtention of 2D MOFs, particularly of Metal-Organic Nanosheets (MONs) has been explored both by bottom-up and top-down approaches [2,3]. In the first case, intricate synthesis conditions or the use of surfactants are required. In the second case, exfoliation of MOFs is limited to architectures that possess strong chemical bonds in two-directions but weaker interactions in the third, dealing as well with low yields and homogeneity.

Herein, we propose the application of Clip-Off Chemistry as a bottom-up-top-down approach to obtain 2D MONs by precise cleavage of double bonds present in known positions of 3D MOFs which contain strong chemical bonds along the three-dimensions of the material. As a proof of concept of this methodology, we took a previously reported MOF, namely LIMF-66 [4], which contains a cleavable tetracarboxylate linker and a non-cleavable tricarboxylate linker. We selectively and quantitatively broke their cleavable linkers through ozonolysis, and successfully obtained novel MONs, which could be characterized by means of Powder X-Ray Diffraction (PXRD) and Scanning Electron Microscopy (SEM). We strongly believe that the use of this methodology further expands the potential for synthesizing and obtaining new materials in this field.



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Keywords: Metal-Organic Frameworks, Metal-Organic Nanosheets.

Design of 2D Germanane Nanoarchitectonics for Implementation in Energy and Biosensing Systems

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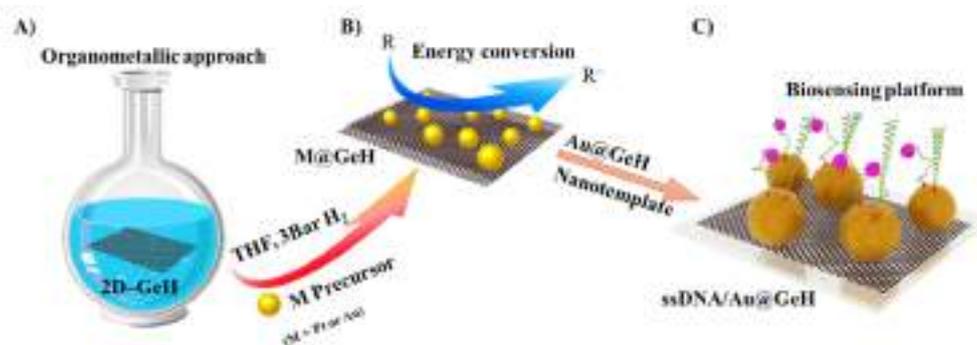
H-terminated 2D–Germanane (2D–GeH), a germanium allotrope akin to graphene, is attracting enormous attention owing to its promising (opto)electronic properties predicted by several theoretical works.^[1] However, the lack of suitable chemical functionalization approaches has hindered its real implementation. Herein, general approaches are developed for the functionalization of 2D–GeH to expand the field of its real implementation.

Firstly, a straightforward organometallic method (**Scheme 1A**) has been utilized for functionalizing 2D–GeH with noble metal nanoparticles (M–NPs), resulting in a new library of 0D/2D M@GeH nanoarchitectonics with appealing electrochemical activity. As a proof-of-principle, both Pt–NPs and Au–NPs have been explored as model noble metals. After an accurate material characterization, the electrocatalytic activity of Pt@GeH and Au@GeH towards two important electrochemical energy conversion reactions —*viz.* hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR)— have been explored (**Scheme 1B**). Compared to the pristine 2D–GeH counterpart, the electrocatalytic HER and ORR performances were enhanced by > 2.5 times when using 0D/2D Pt@GeH and Au@GeH nanoarchitectonics, respectively.^[2]

Beyond electrocatalytic energy conversion, the Au–NPs from 0D/2D Au@GeH nanoarchitectonics were also utilized as nanotemplates for anchoring a thiol-rich single-stranded DNA for the development of robust 2D–GeH-based electrochemical biosensors by taking advantage of the well-known gold–thiol interactions (**Scheme 1C**). In particular, the resulting DNA/Au@GeH material was exploited towards the impedimetric determination of cocaine as a model drug, yielding to a detection limit as low as 4.87 aM. To the best of our knowledge, this is the lowest detection limit found in the literature for cocaine determination.^[3]

Finally, a direct covalent functionalization approach has been pointed out for anchoring molecular components (*viz.* thiolated β -cyclodextrin, CD–SH) onto 2D–GeH. By taking advantage of the CD affinity to accommodate different stereoisomers through supramolecular host–guest interactions, the multitasking activity of the resulting 2D–GeCD has been explored for the selective discrimination of enantiomers and diastereomers.

All in all, the as-developed functionalization approaches result in unprecedented 2D–GeH-based nanoarchitectonics exhibiting outstanding electrochemical properties to expand the practical implementation in advanced electrochemical fields.



Scheme 1. Illustration of the OM approach and its subsequent implementation

Keywords: 2D materials, Germanane, electrochemical sensor, electrocatalysts, Stereodiscrimination

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Synthesis of Spirooxazines with long lifetime of Merocyanine Form

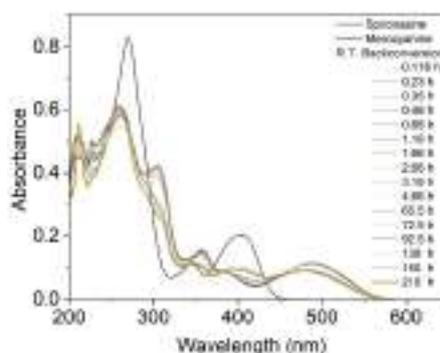
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Keywords: Spirooxazine, energy harvesting, Triplet-state, annihilator design.

In 21st center is interest to chromic compound as spiropyrans, spirooxazines. Different class of compounds able to participate in light-induced reversible transformations. Photochromic compounds is due to photochemical conversion of the initial, the so-called «closed» or spiro- (SP), form to the isomeric merocyanine (MC), or «open», form. [1] The goal of this research is to create of photo-pharmacology compound for use in biomedical applications.[2] Here we report new molecule SO-1 Pic.1 . Which having the longest lifetime of open merocyanine form. Until now we have measured up to 72.5 hr. and only around 35 % has come back at room temperature. The maximum reported lifetime for the open form is 21 min. and it is a bottleneck in Spirooxazine photochemistry studies.



Target molecule SO-1 tested solvent
TX-100 reduced

Figure 5 – Illustration of absorption spectra spirooxazine, back switched stopped 35 %.

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A novel nanotheranostic approach for glioblastoma based on nanocarriers and immuno-PET radiopharmaceuticals (nanothera-PET)

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Introduction: Glioblastoma multiforme (GBM) is the most aggressive primary brain tumor in adults. Epidermal growth factor receptor variant III (EGFRvIII)¹, a specific GBM mutation associated with increased malignancy and poor prognosis, and leukemia inhibitory factor (LIF)², an immunological checkpoint involved in tumor-mediated immunosuppression, are the most attractive ones to develop diagnostic and treatment agents. Due to limitations in current imaging methods for accurate patient stratification and therapeutic monitoring, there is a critical need for improved diagnostic tools. In this regard, immune-PET has emerged as a promising non-invasive imaging technique for the *in vivo* detection of tumor-specific biomarkers. On the other hand, the blood-brain barrier (BBB) presents a major challenge to the effective delivery of this type of diagnostic agents in the initial stages of the pathology before BBB will be disrupted³. In this context, functionalized nanoparticles may offer an innovative strategy to improve BBB permeability. Considering both previous challenges, the goals of this study were: 1) to develop and validate *in vitro* and *in vivo* immuno-PET diagnostic radiopharmaceuticals targeting EGFRvIII and LIF and 2) to assess different nanosystems to perform EGFRvIII targeting and improve the BBB crossing.

Methods: An anti-EGFRvIII and anti-LIF monoclonal antibodies (mAbs) were useful conjugated with the chelating agent deferoxamine (DFO). Quality control was performed by mass spectrometry, gel electrophoresis and SEC-HPLC. On the other hand, extracellular vesicles (EVs) were isolated from EGFRvIII GBM cell lines. Lipid-based nanoparticles (LBNs) were synthesized and functionalized with anti-EGFRvIII and DFO. Both nanosystems were characterized by DLS, NTA and FT-IR. Target affinity studies were performed by flow cytometry and ELISA. Subsequently, radiolabeling of antibodies and nanosystems was carried out with ⁸⁹Zr-oxalate at room temperature. Radiochemical yield, purity and stability of the resulting radioimmunoconjugates were determined by radio-SEC-HPLC and iTLC. The *in vivo* biodistribution of [⁸⁹Zr]Zr-DFO-(mAbs/EV-EGFRvIII/LBN-anti-EGFRvIII) was assessed by PET in an subcutaneous and orthotopic GBM murine models at 24, 48 and 72h post-intravenous administration.

Results: The DFO conjugation of both mAbs was done successfully with 2.4 ± 0.3 DFOs/antibody. In addition, competitive ELISA and flow cytometry assays shown similar affinity of DFO conjugates antibodies than the precursor antibodies. In both cases, the ⁸⁹Zr radiolabeling was done with 99% of radiochemical purity. Concerning preclinical *in vivo* studies in orthotopic GBM murine models by PET/CT, specific accumulation was shown in LIF-released GBM cells (6 ± 1.26 vs 3.01 ± 0.14 %ID/mL) and in EGFRvIII tumor expression (17.19 ± 6.31 vs 1.89 ± 0.24 %ID/mL), with additional uptake in liver, showing hepatobiliary excretion pathway along time. On the other hand, ⁸⁹Zr radiolabeling was done for EVs and LBNs functionalized nanoparticles with 99% of radiochemical purity. PET/CT molecular imaging experiments were done in subcutaneous GBM model, showing proper tumor uptake in both cases: EV-EGFRvIII (13.34 ± 2.10 vs 9.19 ± 0.54) and LBN-anti-EGFRvIII (10.93 ± 2.78 vs 3.23 ± 0.85 %ID/mL).

Conclusions: [⁸⁹Zr]Zr-DFO-anti-LIF, [⁸⁹Zr]Zr-DFO-anti-EGFRvIII, [⁸⁹Zr]Zr-DFO-EV-EGFRvIII and [⁸⁹Zr]Zr-DFO-LBN-anti-EGFRvIII was successfully synthesized and demonstrated promising *in vitro* and *in vivo* target-binding properties for using as diagnostic agents. This approach integrates molecular imaging and nanotechnology, paving the way for personalized medicine in GBM management.

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