

DOCTORAL WORKSHOP

PhD in Chemistry

Scientific Programme and Book of Abstracts

May 23rd-24th 2024

Sala d'Actes

Faculty of Science

Organised by the Department of Chemistry

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

May 23rd-24th 2024

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, 14 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



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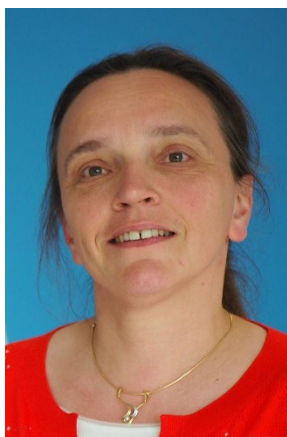
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INVITED SPEAKERS

Prof. Veronique Van Speybroeck
Ghent University

Veronique Van Speybroeck is full professor at the Ghent University and head of the Center for Molecular modeling (<http://molmod.ugent.be>), a multidisciplinary research center composed of about 40 researchers. She was trained as an engineer in Physics and obtained her PhD in 2001 from the Ghent University. She has a record of [significant contributions](#) in the field of modeling nanoporous materials for catalysis, adsorption; all applications are inspired and performed in close synergy with experimental groups. The research is driven by the ambition to model as close as possible realistic materials/processes and systematically pushed the limits of simulation methods. She developed methods to calculate chemical kinetics for reactions taking place in nanoporous materials and pioneered the simulation of complex catalytic cycles at operating conditions using enhanced sampling molecular dynamics methods. Currently, she is exploring methods to resolve complex catalytic cycles bridging length and time scales. She was recipient of two ERC grants, received numerous recognitions and prizes, such as the [Dr. Karl Wamsler innovation award in 2023](#). She is also an elected member of the Royal (Flemish) Academy for Science and the Arts of Belgium (KVAB, www.kvab.be).

Prof. Alberto Escarpa
University of Alcalá de Henares

Alberto Escarpa is a Full Professor of Analytical Chemistry at the University of Alcalá. His main research interests are microfluidics and micromotors for (bio)sensing. He has co-authored more than 200 articles in leading journals, books, and book chapters (h-index of 50). He has been included in the top 1% of most cited chemists worldwide (2020, 2021 by Stanford University). His works have been highlighted in top journals and social scientific media. He has given more than 50 invited lectures. He has received several awards such as the NATO Fellowship to perform postdoctoral research at the New Mexico State University (USA) in 2001, the "Young Investigator Award" by the University of Alcalá in 2003, the International Dropsens Award "Best Research Work in applied electroanalytical chemistry" (finalist) in 2015, the Excellence Award in Doctoral Thesis Direction of Sciences in 2021 at University of Alcalá, and Spanish Royal Society of Chemistry Award for Research Excellence 2024. He is currently a member of the Editorial Board of Analytical Chemistry and Editor in Chief for Microchimica Acta.



Dr. Beatriz Pelaz
University of Santiago de Compostela



Beatriz Pelaz received her PhD from the University of Zaragoza in 2012. From June 2012 to December 2016, Beatriz was a member of Professor Wolfgang J. Parak's group at Philipps-Universität Marburg in Germany, first as a postdoctoral researcher and later as a Humboldt researcher.

Since January 2017, she has co-led the BioNanoTools group at CiQUS, initially as the principal investigator of a project for young researchers (JIN, MINECO), later as a Ramón y Cajal researcher (2017 call, affiliated with the Inorganic Chemistry department of the University of Santiago de Compostela). Currently, she is an Associate Professor at the USC. In 2020, the

European Research Council awarded her a Starting Grant. Since 2021, she is member of the Young Academy of Spain.

Her research focuses on developing remotely controllable smart materials and their interaction with biological entities.



SCIENTIFIC PROGRAM

May 23rd**09:00—09:15 Welcome and opening**

Prof. Lluís Escriche, Head of the Department of Chemistry

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

09:15—10:15 Plenary Lecture

Chairman: Xavier Solans

Title: Operando modelling of functional nanostructured materials for future technologies
Prof. Veronique Van Speybroeck

10:15—11:15 Poster session + Coffee Break**11:15—12:45 Presentations I**

Chairwoman: Maria Jesús Sánchez

- 11:15 - 11:30** Is Size All That Matters? A Discussion on the Functionalisation of Metallic Nanoparticles. **Álvaro Lozano Roche**. P1.1
- 11:30 - 11:45** Investigating CO₂ Formation on Interstellar Water Ice: A Computational Study. **Harjasnoor Kakkar**. P1.2
- 11:45 - 12:00** Giant oligomeric porous cage-based molecules. **Alba Cortés Martínez**. P1.3
- 12:00 - 12:15** Structure-based design of serotonin 5-HT_{2C} receptor positive allosteric modulators for the treatment of obesity. **Aleix Quintana García**. P1.4
- 12:15 - 12:30** Synthesis and photochemical characterization of new Smart UV filters. **Cristina Moya Muñoz**. P1.5
- 12:30 - 12:45** Electrolyte Gated Organic Field Effect Transistors for Point-Of-Care Tests. **María Jesús Ortiz Aguayo**. P1.6

12:45—15:00 Break**15:00—16:00 Plenary Lecture**

Chairman: José Muñoz

Title: Micromotors in action as smart microsensors: just a concept or a reality?
Prof. Alberto Escarpa

16:00—17:00 Presentations II

Chairwoman: Carolina Gimbert

- 16:00 - 16:15** Fluorine meets visible-light: sustainable methods and tunable materials. **Albert Gallego Gamo**. P2.1
- 16:15 - 16:30** Rapid screening test for Streptococcus agalactiae neonatal infections combining portable PCR and electrochemical. **Anaïxis Del Valle Peña**. P2.2
- 16:30 - 16:45** Development of a new PEG-based biocompatible sealant for surgical applications. **Alba López Moral**. P2.3
- 16:45 - 17:00** Improvement of cocaine electrochemical detection with tailor-made polymers. **Elena Rodríguez Franch**. P2.4



May 24th

09:30—10:30 Presentations III

Chairman: Xavier Sala

- 09:30 - 09:45** Engineering of Glioblastoma-derived Biomimetic Vesicles. **Noelia Hernández Lobato**. P3.1
- 09:45 - 10:00** Multivariate Metal-Organic Frameworks: Quest for Complexity. **Xiao Bao Li**. P3.2
- 10:00 - 10:15** Lignocellulosic biomass conversion into biochemicals using pyrolysis. **Mireia Mora Sanjuan**. P3.3
- 10:15 - 10:30** Co-assembly of Polyhedral Metal-Organic Framework Particles into Binary Ordered Superstructures. **Lingxin Meng**. P3.4

10:30—11:30 Poster session + Coffee Break

11:30—12:30 Plenary Lecture

Chairwoman: Rosario Núñez

Title: Development of efficient nanocarriers
Dr. Beatriz Pelaz

12:30—12:45 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

PhD STUDENTS



Is Size All That Matters? A Discussion on the Functionalisation of Metallic Nanoparticles

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K. Philippot²; J. García-Antón¹; X. Sala¹

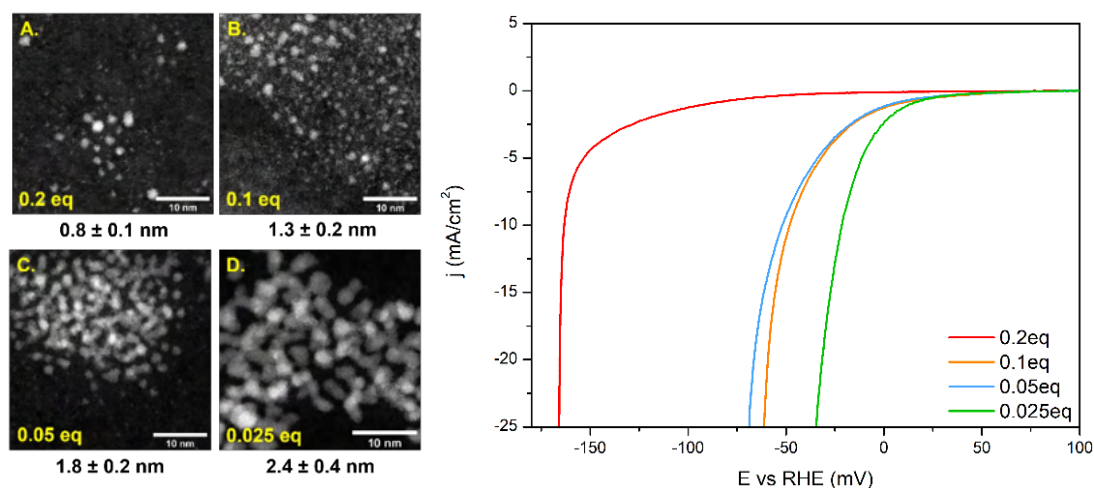
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In recent years metallic nanoparticles (NPs) have increased their popularity for numerous catalytic applications. This is largely due to their size-related properties. When compared to typical homo- and heterogeneous catalysts, metallic NPs gather some of the best properties of both worlds.^[1] One particularly interesting method for the synthesis of metallic NPs is the organometallic approach. This procedure entails the controlled decomposition of an organometallic precursor in the presence of a stabiliser, usually a ligand of interest, under mild conditions. In this way, the synthesised NPs present a clean surface free of contaminant by-products.^[2] Interestingly, the ligands attached to the surface of NPs have been shown to alter the physicochemical properties of the system and even increasing their catalytic efficiency, as in the case of Ru NPs stabilised with 4-phenylpyridine ligand for HER.^{[3], [4]} Herein we present various systems consisting of Ru NPs stabilised with different amounts of 2,2'-bipyridine (bpy). It was found that there is an inverse relationship between the amount of bpy used and the NP size. These differences in size also translate into their catalytic performances towards HER, being the smallest system the worst and the biggest one the best. This behaviour can be justified by the effect of the bpy ligand on the active sites of the NPs by combination of experimental (electrochemistry, XPS, synchrotron) and computational studies.



Keywords: Nanoparticles, Catalysis, Electrochemistry, Artificial Photosynthesis

References:

- [1] P. Serp, K. Philippot, in *Nanomaterials in Catalysis* (Eds.: P. Serp, K. Philippot), Wiley-VCH, Weinheim 2013, 1-54.
- [2] C. Amiens, D. Ciuculescu-Pradines, K. Philippot, *Coordination Chemistry Reviews* 2016, 308, 409-432.
- [3] J. Creus, S. Drouet, S. Suriñach, P. Lecante, V. Collière, R. Poteau, K. Philippot, J. García-Antón, X. Sala, *ACS Catal.* 2018, 8, 12, 11094-11102.
- [4] G. Martí, L. Mallón, N. Romero, L. Francàs, R. Bofill, K. Philippot, J. García-Antón, X. Sala, *Adv. Energy Mater.* 2023, 2300282.



Investigating CO₂ Formation on Interstellar Water Ice: A Computational Study

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Solid CO₂ has been detected in various physical environments in the interstellar medium (ISM) since its first observation in 1989.[1] Despite being one of the most abundant species in the ISM and a significant component of ice mantles on dust grains, the formation route of CO₂ remains uncertain.[2] The low abundance of CO₂ in the gas phase suggests that it is exclusively formed on the solid ice surface. Moreover, there is no clear, efficient process that can account for the majority of CO₂ formation.[3] In this study, we investigate three well-known radical-neutral reaction pathways (CO with O, CO with OH, and HCHO with O) on pure water ice clusters using quantum chemical calculations. Multiple density functional theory (DFT) functionals are employed to carry out the preliminary benchmarking study on the model gas-phase reactions and determine an accurate method for describing the reaction properties. With the selected functional, potential energy surfaces of the reactions are obtained on ice models i.e., two water clusters consisting of 18 and 33 molecules. First insights will be presented based on the computational investigation that aims to determine the energetically feasible reaction mechanisms. The astrophysical implications of the results will be discussed in combination with observations from experiments and astrochemical models of these widely studied reactions.

Keywords: Interstellar Medium; Surface Ices; Interstellar Dust Processes; Computational Methods

References:

- [1] J. E. Roser, G. Vidali, et al. *Formation of carbon dioxide by surface reactions on ices in the interstellar medium*, *Astrophys. J.* 555, L61-L64 (2001)
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- [3] R. T. Garrod, T. Pauly, *On the formation of CO₂ and other interstellar ices*, *Astrophys. J.* 735, 15 (2011)



Giant oligomeric porous cage-based molecules

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The majority of known porous materials are either small (< 5 nm) discrete cages (i.e. coordination and covalent cages), or infinite networks (i.e. metal- and covalent-organic frameworks). The chemical and dimensional (between 5 nm and 20 nm) space between these two classes has not been largely explored, due to the inherent synthetic and analytical challenges.^{1,2,3}

In this communication, it will be described a new strategy for the stepwise synthesis of oligomeric porous molecules by the concatenation of a defined, finite number of porous units. To this end, metal-organic polyhedra (MOPs)⁴ have been used as monomers to form three new oligomeric molecules through azide-alkyne cycloaddition click chemistry (Figure 1).

The resultant giant oligomeric porous molecules can potentially merge the properties that arise from linking pore units (i.e. extrinsic porosity and inter-cavity cooperativity) to the those typically observed in molecules, such as defined molecular weight, stoichiometric reactivity, and solubility in liquids.

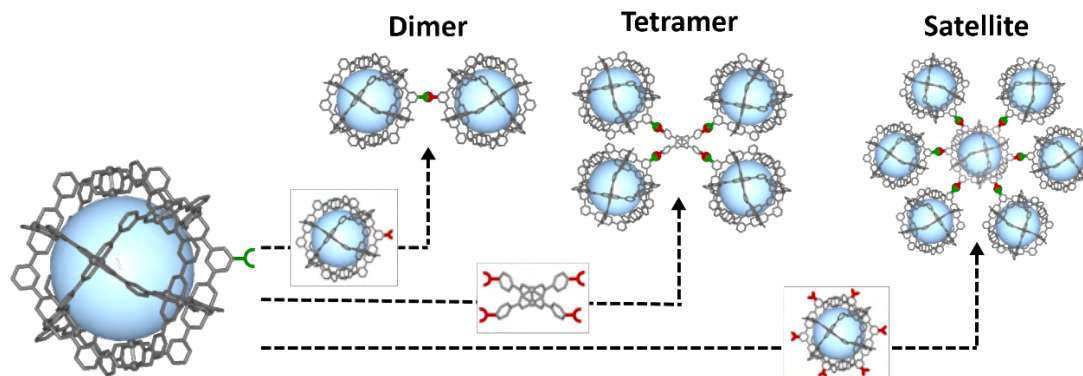


Figure 1. Schematic of the use of a metal-organic polyhedra to synthesise giant oligomeric cage-based molecules.

Keywords: Meta-organic polyhedra, cages, porous molecules, oligomeric materials and click chemistry.

References:

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Structure-based design of serotonin 5-HT_{2C} receptor positive allosteric modulators for the treatment of obesity

A. Quintana[†], L.A. Howell[‡], A. González[†], P.J. McCormick[‡], O. Illa[†], L. Pardo^{†,*}

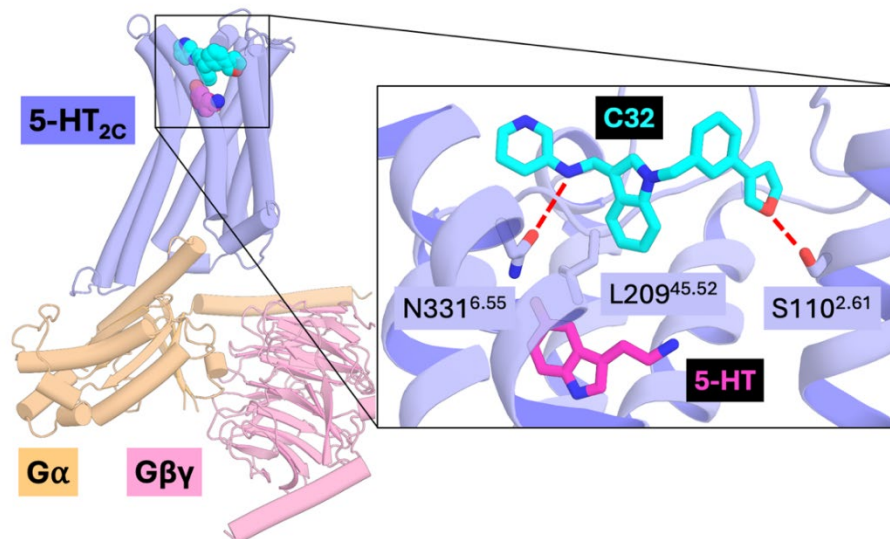
[†]Laboratori de Medicina Computacional, Unitat de Bioestadística, Facultat de Medicina and Unitat de Química Orgànica, Departament de Química, Facultat de Ciències, Universitat Autònoma de Barcelona

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The serotonin 5-HT_{2C} G protein-coupled receptor (GPCR) subtype has been increasingly investigated as a therapeutic target for the treatment of obesity and substance use disorders (SUDs).¹ Historically, 5-HT_{2C} agonists, such as the FDA-approved lorcaserin, have been employed in anti-obesity treatment given that 5-HT_{2C} is a critical mediator in food intake and body weight control during serotonergic activation.¹⁻³ However, receptor subtype selectivity is a major determining factor in their therapeutic utility, as the activation of the highly homologous 5-HT_{2A} and 5-HT_{2B} can lead to hallucinations and cardiac valvulopathies, respectively.¹⁻³ In recent years, the use of positive allosteric modulators (PAMs) as an alternative therapeutic strategy has shown promise.⁴ These compounds act on topologically distinct sites from the orthosteric site, offering improved selectivity while mitigating the adverse effects of chronic exposure to orthosteric ligands. In this work, we disclose a series of novel 5-HT_{2C} PAMs evolved from the study of the previously reported VA012⁵ within the context of the 5-HT_{2C} cryo-EM structure.⁶ These compounds exhibited an improved dose-dependent enhancement of serotonin efficacy compared to its predecessor. We provide mechanistic insights into their recognition mode and pharmacodynamic profiles using computational models and mutagenesis experiments.

Keywords: 5-HT_{2C} receptor, PAMs, obesity, MD simulations, mutagenesis.



References:

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4. Persechino, M. et al. *Pharmacol. Ther.* 237, 108242 (2022).
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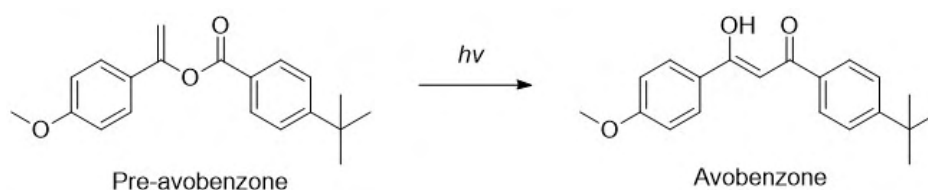
Synthesis and photochemical characterization of new Smart UV filters

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Excessive exposure to ultraviolet (UV) radiation from sunlight is known to cause various damaging effects on the skin, including sunburns¹, premature aging², and an increased risk of certain types of skin cancer³. To mitigate these risks and protect the skin, the application of sunscreen is essential. Sunscreens can be categorized into chemical and physical types, which either absorb or reflect UV radiation⁴, respectively. A few years ago a new generation of UV chemical filters was developed (Smart UV filters) that are characterized by a progressive enhancement of their sun filtering effect under solar irradiation.⁵ This behaviour is achieved by progressive phototransformation of the initial smart UV filter (e.g., pre-avobenzone, Scheme 1) into a more efficient sunscreen (avobenzone) upon UV radiation. As a result, this process enables prolonged and adjustable solar protection during sunlight exposure.



Scheme 1. Phototransformation of pre-avobenzone after irradiation with UV light

The present study focuses on the synthesis and characterization of new progressive sun filters derived from pre-avobenzone analogs, aiming to enhance their photochemical properties, particularly in terms of UVB absorption. Computational analyses of the absorption spectra for various pre-avobenzone derivatives and their photoproducts were conducted to identify promising candidates for further investigation. Subsequently, a selection of these compounds was synthesized and subjected to detailed photochemical characterization to evaluate their efficacy as progressive sun filters. Notably, one compound exhibited superior performance compared to the original pre-avobenzone, demonstrating enhanced UV protection capabilities, before and after irradiation. Furthermore, the structural modifications influencing the phototransformation process were rationalized based on detailed photochemical measurements.

Keywords: ultraviolet radiation, sunscreen, UV absorption, Smart UV filters, phototransformation

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- ⁴ Egambaram, O. P.; Kesavan Pillai, S.; Ray, S. S. *Photochemistry and Photobiology*, **2020**, *96*, 779–797.
- ⁵ Gallardo, A.; Teixidó, J.; Miralles, R.; Raga, M.; Guglietta, A.; Marquillas, F.; Sallarès, J.; Nonell, S. *Photochem. Photobiol. Sci.* **2010**, *9*, 530–534.



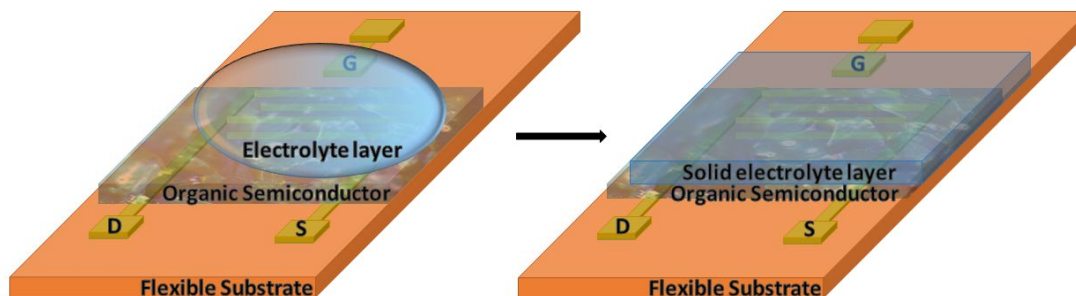
Electrolyte Gated Organic Field Effect Transistors for Point-Of-Care Tests

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Over the last few years, flexible electronics are resonating in a wide variety of novel (bio)applications. As a key device, electrolyte-gated organic field-effect transistors (EGOFETs) are raising considerable interest due to their inherent advantages on miniaturization, low cost fabrication using solution – processing methods, low power consumption and label - free transduction, among others. Bearing this in mind, we manufacture a novel EGOFET replacing the liquid electrolyte for solid-electrolyte platforms (i.e. Hydrogels). These electrolytes could overcome the limitations that aqueous media presented provide good mechanical properties and excellent biocompatibility. In addition, hydrogels offer a suitable environment for the immobilization of biomolecules. The experimental approach involves the fabrication and characterization of EGOFETs using an organic semiconductor (OSC) as the active material and different electrolyte media. For this reason, we fabricated EGOFETs using a processing technique compatible to roll – to- roll processes (i.e. Bar-assisted meniscus shearing (BAMS)) which allows the deposition of a layer of OSCs blended with polystyrene (PS). Subsequently, the devices were characterized electrically by means of Transfer and Output Characteristics, in order to demonstrate that the electrical parameters between devices with solid and liquid electrolytes are comparable. Our work demonstrates that the fabricated EGOFETs using hydrogels exhibit comparable electrical performance and long-term stability regarding those employing liquid electrolytes, and therefore, they could be employed in several applications such as sensors of (bio)analytes of interest and Point-of-care (POC) devices. In conclusion, this research underscores the promising prospects of EGOFETs in transforming point-of-care testing. The integration of organic semiconductors and electrolyte gating not only enhances device sensitivity but also offers cost-effective and portable solutions for diagnostic applications. Future research may further refine and expand the application of EGOFETs, paving the way for widespread adoption in routine diagnostic practices.

Keywords: Organic Electronics, EGOFET, Biosensing, POC testing, solid electrolyte.





Fluorine meets visible-light: sustainable methods and tunable materials

A. Gallego-Gamo, R. Pleixats, A. Granados, C. Gimbert-Suriñach,* A. Vallribera.*

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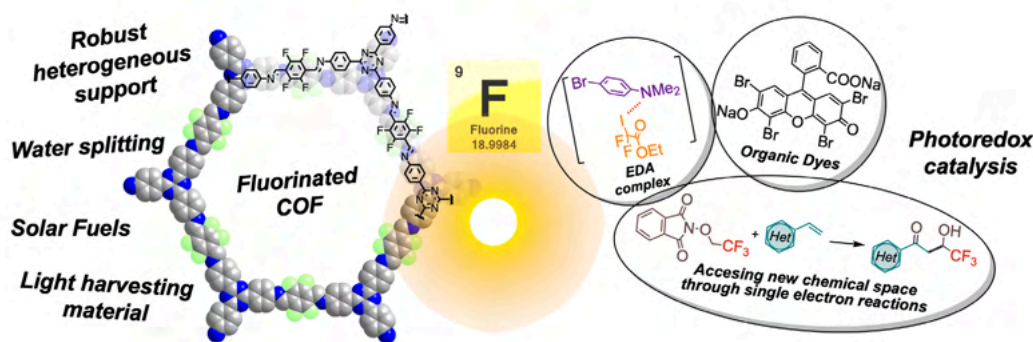
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In recent years organofluorine chemistry has had a great impact on scientific research, academia, and industry due to its fascinating features and wide applications. Among them, its emergence in the synthesis of functional materials or its incorporation in biologically active skeletons have been of utmost importance. The presence of fluorine in organic molecules and materials allowed them to exhibit unprecedented properties in contrast to their non-fluorinated counterparts.^[1]

Nowadays, the energy supply for humanity is problematic. Therefore, the design of new sustainable platforms is a requirement for researchers. In this scenario, the use of visible-light as an energy source is emerging as a true replacement for non-renewable feedstocks. The progress in artificial photosynthesis to obtain H₂ or the use of photocatalysis to drive synthetic modifications are a couple of examples of its implementation in the chemistry field.^[2,3]

Based on the approach that chemical research is achieving and the background that our group offers, our current research lines are focused on i) the synthesis of fluorinated functional materials and study its use in sustainable synthetic platforms; ii) taking advantage of photocatalysis as a tool for the functionalization and fluorination of small molecules.^[4-7]

On the one hand, the synthesis of trifunctional fluorinated molecules and their use as monomers in the preparation of Covalent Organic Frameworks (COF) is described. Studies of the structural, spectroscopic and electronic properties of the resulting materials are proposed to observe the influence of fluorine. Finally, their use as heterogeneous support or photosensitizer on different catalytic platforms is presented. On the other hand, new photoredox methods for the (fluoro)alkylation of organic backbones have been accomplished. A broad range of new molecules with medical relevance is presented along with a deep study regarding the mechanism of the transformations.



Keywords: Organofluorine Chemistry, Covalent Organic Frameworks, Photocatalysis, Electron Donor Acceptor (EDA) Complex.

References:

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Rapid screening test for *Streptococcus agalactiae* neonatal infections combining portable PCR and electrochemical genosensing

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Streptococcus agalactiae (Group B Streptococcus, GBS) is the primary cause of neonatal infections affecting pregnant mothers and, particularly, their offspring. This infection affects 18% of pregnant women globally (rising to 35% in certain regions), leading to a range of diseases, including maternal infection, stillbirth, and early- and late-onset sepsis in newborns. Additionally, GBS may contribute to preterm delivery and hypoxic ischemic encephalopathy. In 2020, an estimated 90,000 infant deaths were attributed to GBS, with nearly half of these occurring in Sub-Saharan Africa. To mitigate these alarming statistics, proactive administration of preventive antibiotics to the mother during delivery is initiated upon positive detection of GBS (typically around week 36 of pregnancy). This measure aims to prevent vertical transmission during childbirth and minimize risks to the baby. However, current detection methods rely on culturing techniques, resulting in long turnaround times for results and requiring sophisticated laboratory infrastructure and training. Diagnosing GBS in newborns is even more challenging, as it requires a minimum volume of blood and/or cerebrospinal fluid for successful culture, which can be difficult to obtain from these patients. Moreover, the time required for obtaining results can span several days. Given these limitations, this PhD thesis addresses the development of a point-of-care rapid screening test based on a handheld thermocycler to perform double tagging endpoint PCR. Accordingly, a conventional PCR with a novel thermostable DNA polymerase, primer design and testing of a GBS-specific gene, screening of several bacterial lysis methods, methodology specificity determination, and Limit of Detection were performed. The development of this doctoral dissertation holds the potential to improve current protocols for GBS infection detection, allowing for rapid point-of-care screening both in expectant mothers and at the newborn's side. Such a breakthrough could significantly reduce the global burden of GBS disease, with impact in low-income countries due to the challenges of implementing microbiological cultures in these settings.

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Development of a new PEG-based biocompatible sealant for surgical applications

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During surgeries, sutures, staples, and clips are commonly utilized. However, these methodologies are slow, lack precision, and can cause additional tissue damage. To address these limitations, sealants have been developed. For effective application, these sealants must exhibit biocompatibility, strong adhesion in wet biological substrates, and suitable biodegradation properties. Polyethylene glycol (PEG)-based sealants have attracted considerable attention in biomedical research due to their ability to enhance material biocompatibility, facilitating versatile applications in tissue engineering and surgical interventions. Typically, these sealants exhibit burst pressures ranging from 10 kPa to over 100 kPa in preclinical studies, with variations influenced by factors such as crosslinking density, molecular weight of PEG chains, and tissue substrate. While several PEG-based sealants are available in the market, they are primarily used for suture reinforcement. Hence, we propose the development of new biocompatible PEG-based sealants, with rapid curing times and superior self-adhesion properties.

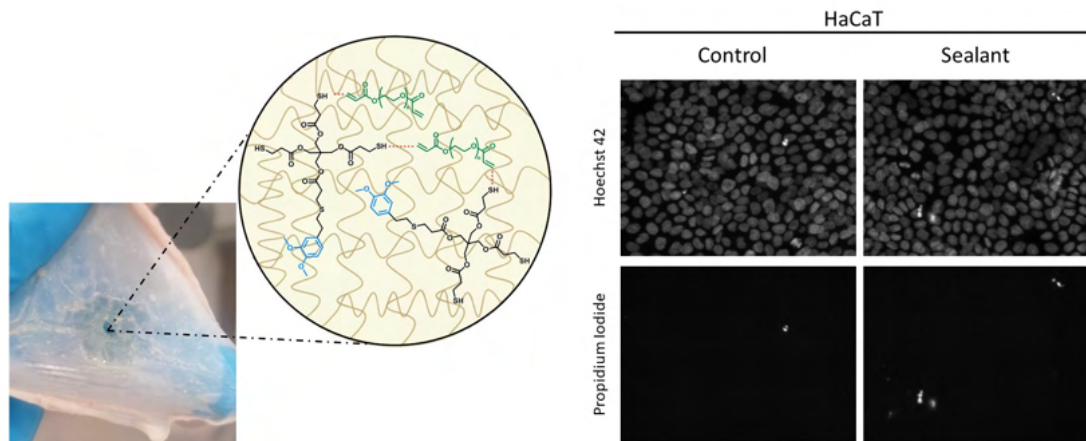


Figure 1. A) Schematic representation of the bonds created during the curing process of the sealant over the intestine tissue. B) Keratinocytes (HaCaT) pictures of the viability tests. Hoechst 42 filter shows all the cells while Propidium Iodide elucidates only the dead ones.

We suggest the use of thiol-ene reaction for the crosslinking process due to its rapid nature, resulting in shorter curing times. To achieve this, we propose a formulation comprising three components: diacrylate PEG chains for biocompatibility and adhesive properties, thiolated derivatives serving as crosslinking and doping points, and a photo-initiator, which should exhibit absorbance in the visible range to ensure safety during irradiation. The material is represented in Figure 1 A.

Hence, we obtained a formulation composed of the diacrylate PEG MW 700, 3,4-Dimethoxystyrene and BAPO, that irradiated at 430 nm gave burst pressures of 29.57 ± 2.58 kPa in porcine skin without previous suture and any influence in the cell viability (see Figure 1 B).

Keywords: sealant, PEG, photopolymerization, thiol-ene reaction.

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Improvement of cocaine electrochemical detection with tailor-made polymers

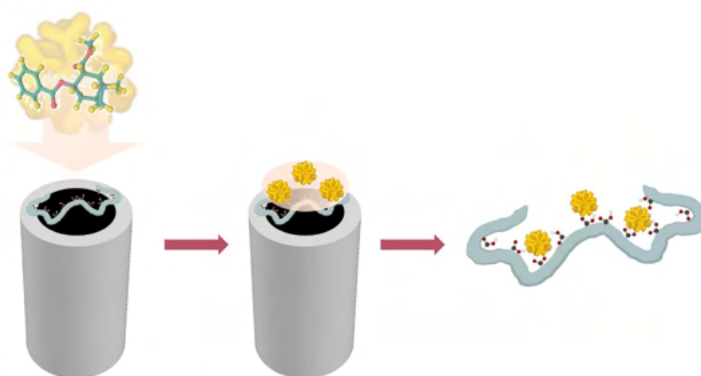
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In view of the increasing use of international borders as gateways for illicit drugs and their precursors, law enforcement authorities require new analytical tools capable of achieving the rapid detection of illicit drugs [1-3]. There is great interest in the development of new portable and wireless devices that can reliably and sensitively detect these substances at trace level [4]. The main challenges of the current in-situ methods used are the low accuracy for color tests and the high cost and limited portability for spectroscopic testing. In response to these challenges, BorderSens project aims to establish the basis for the development of a unique, portable and wireless device capable to quickly test different drugs, precursors and cutting agents, with improved sensitivity and specificity. This project combines the inherent advantages of electrochemical sensors, molecularly imprinted polymers, multivariate data analysis and pattern recognition tools.

Herein we present an overview of some of the achievements made so far in the detection of cocaine and some of their common cutting agents. Some of them, i.e., levamisole showed a suppression effect on the signal of cocaine, which might cause false negative results. Two strategies were proposed to avoid this suppressing effect and reveal the signal of cocaine on un- modified graphite epoxy composites (GEC) electrodes. First, the adjustment of the pH of the detection solution to pH 12 and applying a cathodic pretreatment. Besides, another strategy involves the modification of GEC electrodes with affinity polymers for cocaine. These sensors achieved limits of detection in the μM range.

The usefulness of electrochemical techniques in predicting possible interfering agents has been successfully demonstrated. With the major advantages of superior specificity, speed, simplicity, and low cost, the developed strategies offer a promising alternative for on-site screening of seized cocaine samples.



Keywords: illicit drugs, cocaine, levamisole, electrochemical sensors, molecularly imprinted polymers.

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Engineering of Glioblastoma-derived Biomimetic Vesicles

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In the last decade, the development of biomimetic nanosystems has emerged as a new strategy to engineer novel vesicular transport systems for a variety of therapeutic applications. The ‘biomimetic’ concept relies on the incorporation of cell membrane components as integral parts of the vesicles, conferring them with biological properties originating from the cell of origin. The different design strategies of biomimetic nanosystems can be distinguished in two broad categories: **i)** cell-membrane wrapped (pre-formed) nanoparticles; and **ii)** cell-derived lipid vesicles, containing either mixture of all cell-membrane components or selected protein components. The majority of studies published today focus on the evaluation of the biological activity and function of the different biomimetic nanosystems with limited engineering and formulation details of the methodology used.

This study focuses on the engineering of biomimetic lipid vesicles by incorporation of murine glioblastoma cell (GL261) extracted proteins only, using classical liposome fabrication methodologies (lipid film hydration and extrusion). We evaluated different vesicle engineering parameters, including, cholesterol content, degree of PEGylation, as well as some processing aspects like purification and quantification. Both the cholesterol concentration and degree of PEGylation played an important role in the size and monodispersity of the biomimetic vesicle populations. The biomimetic GL261-derived vesicles were purified using size exclusion chromatography in combination with other solid-phase purification techniques to ensure the separation between the unbound proteins and the GL261-derived vesicles. After obtaining the purified systems, the GL261-derived vesicles were characterized structurally by cryo-EM and differential scanning calorimetry (DSC), while their molecular protein profile was evaluated using mass spectroscopy (LC-MS/MS).

We elucidate valuable insights on the importance of various molecular and methodological parameters for the fabrication of monodisperse and colloidal stable GL261-derived biomimetic vesicles, and their impact on the resultant overall vesicle morphology, thermal properties and protein content. Such information is critical in informing the further therapeutic use of such engineered vesicles.

Keywords: biomimetic vesicles, liposomes, glioblastoma, membrane proteins, personalized therapy.



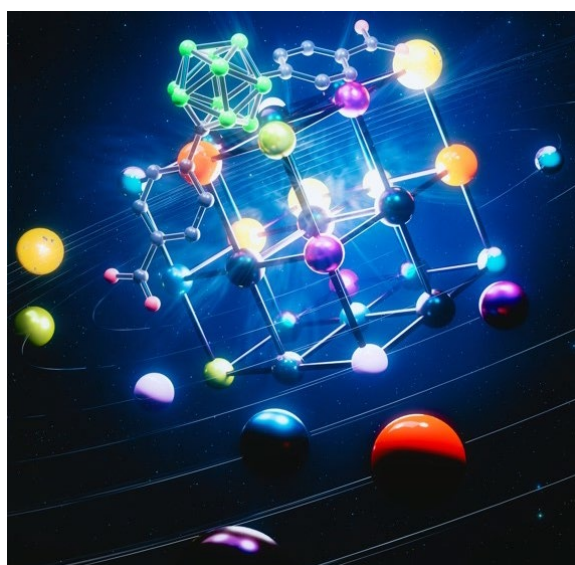
Multivariate Metal-Organic Frameworks: Quest for Complexity

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Currently, the focus of research on metal-organic frameworks (MOFs) is transitioning from understanding the basic principles governing their assembly, structure, and porosity, towards more intricate concepts that utilize chemical complexity to engineer new functions and properties. This shift embraces the synergy of different components within these networks, leading to the development of multivariate (MTV) MOFs.¹ Overall speaking, the deliberate combination of different connectors and metals is a necessary way to program the development of new functional materials. We have recently reported a new type of multi-metallic MTV-MOFs combining a hydrophobic *m*-carborane linker (*m*CB-L) and rare earth (RE) cations (La, Ce, Eu, Gd, Tb, Dy, Y, and Yb), which can incorporate up to 8 different RE cations with different sizes and equimolar amounts and no compositional segregation.² Demonstration of the incorporation of all RE cations is performed via compositional and structural characterization. We will discuss these results and our ongoing studies on multi-metallic transition metal MTV MOFs with our carborane based linkers.



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Lignocellulosic biomass conversion into biochemicals using pyrolysis

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The pressing need for fossil fuel replacement in today's society is driving research into alternative renewable feedstocks and energy sources. Forestry biomass plays a key role in the development of bioeconomy, providing a non-food competitive source of valuable chemicals. In this work, which is encompassed inside the European project LIFE BIOEFFORMED, an innovative strategy to produce renewable value-added chemicals and biofuels was developed, using a semi-industrial torrefaction and pyrolysis plant to produce bio-oil, biochar and gas from wood. These intermediates were further processed and turned into biochemicals and bioproducts.

Different types of lignocellulosic biomass were used and compared to produce bio-oil, biochar and gas. In this study bio-oil was further refined with biorefinery techniques like vacuum distillations, liquid-liquid extractions and column chromatography to separate value-added chemicals such as sugars (e.g. levoglucosan), carboxylic acids (mainly acetic acid) and antioxidants like catechol, guaiacol, vanillin and many others [1,2].

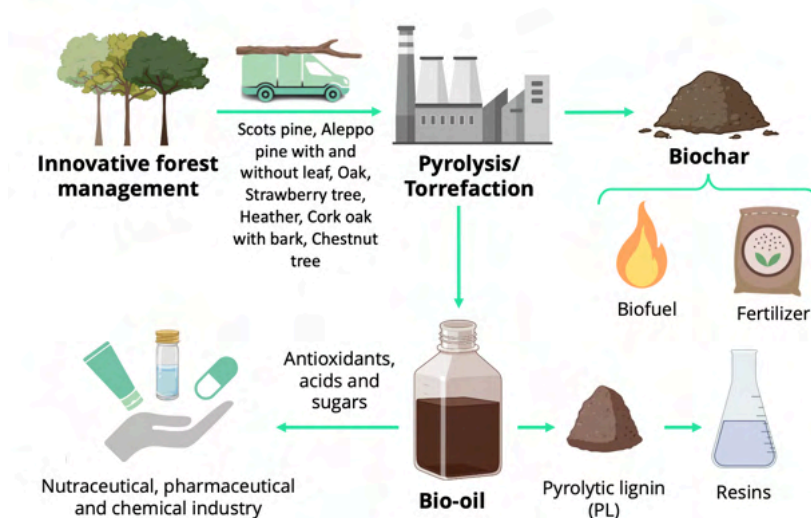


Figure 2. Transformation of lignocellulosic biomass into bioproducts.

Keywords: Bioeconomy, Biomass, Bio-oil, Biorefinery, Pyrolysis

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Co-assembly of Polyhedral Metal-Organic Framework Particles into Binary Ordered Superstructures

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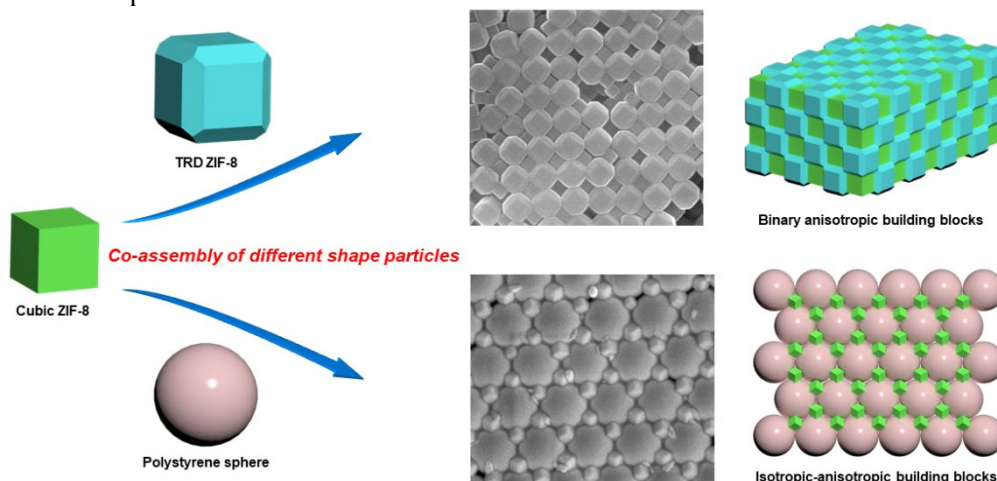
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Self-assembly of colloidal particles into ordered three dimensional (3D) superstructures offers novel opportunities for producing functional materials with photonic, magnetic, electronic, catalytic, mechanical, and thermal properties, owing to their collective spontaneous organizational behaviour.¹⁻³ Traditionally, isotropic particles have been used to generate binary co-assemblies;⁴ however, superstructures made of two different polyhedral particles remain very scarce. Here, we will show the utilization of colloidal polyhedral metal-organic framework (MOF) particles with complementary sizes and shapes to create 3D binary superstructures. As a proof of concept, we have demonstrated the formation of a face-centered cubic (fcc) NaCl-type porous superstructure through the co-assembly of oppositely charged truncated rhombic dodecahedral ZIF-8 particles and cubic ZIF-8 particles. As well, we have co-assembled binary ordered superstructures from cubic ZIF-8 particles and spherical polystyrene (PS) particles. The simplicity and versatility of our assembly approach may facilitate the on-demand manufacture of sophisticated superstructures integrating particles with a wide range of sizes, shapes, and chemical compositions.



Keywords: Self-assembly, Metal-Organic Framework, ZIF-8, superstructure.

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