ChIR Symposium 2024

Universitat de Barcelona

8th and 9th July

Chemical Regulation and Innovation for Sustainable Development

Book of Abstracts

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Welcome to the ChIR Symposium, 2024!

Chemical Regulation and Innovation for Sustainable Development

We are thrilled to invite you to the ChIR Annual Symposium 2024, which will be held in the vibrant city of Barcelona on July 8 and 9, 2024. This year's theme is "Chemical Regulation and Innovation for Sustainable Development," reflecting our commitment to fostering dialogue and collaboration among students, researchers, and industry professionals.

The ChIR Annual Symposium 2024 aims to bridge the gap between advancements in chemical safety regulations and the innovative processes driving sustainability in the chemical industry. Our focus will be on the critical intersections between regulatory frameworks, technological innovation, and the United Nations' Sustainable Development Goals (SDGs).

Table of Contents

Symposium Programme Timetable

Monday, July 8

09:00	Registrations		
09:30	**Opening session**		

Session 1 Environmental Sustainability

Chairperson: *Emilio Tagliavini*

09:40	**Keynote 1**	Angelo Romasanta (ESADE)	Management of Innovation in Chemical Sustainability
10:20	**TP1**	Bryan Leonardo Morales Espino	Lycopene extraction from tomato waste using sustainable solvents
10:30	**TP2**	Jordi Falguera Garcia	Development of 4th generation batteries quality control in the lamination process
10:40	**TP3**	Breno Savazini Leone	Redesigning polyurethane cavity filling acoustic foam for increased safety and sustainability
10:50	**TP4**	Bositkhon Akhmedov	Development of green chitin-based materials for thermal insulation and packaging applications
11:00	*Discussion*		
11:20	**Coffee break**		
11:40	*Poster Session*		

Session 2 Green Synthesis and Catalysis

Chairperson: *Isabel Cavaco*

11:50	**TP5**	Alex Kamande	Cyclopalladated of α-amino acids Schiff bases and their application in Suzuki reactions
12:00	**TP6**	Ayoub Antar	Synthesis of magnetic hybrid core@shell nanomaterials: Fe_3O_4 nanoparticles coated with spin crossover polymer
12:10	**TP7**	Perfect Peace Sunday	New catalyst for CO_2 conversion via Reverse Water-Gas Shift process
12:20	**TP8**	Raphael Mensah	Study of MAX phases and 2D-derived materials for CO_2 conversion through the reverse water gas Shift reaction
12:30	*Discussion*		
12:50	**TP9**	Samuel Amali	Microwave-Assisted Synthesis of Heterometallic Lanthanoid 2D Metal-Organic Frameworks.
13:00	**TP10**	Gavrilla Anggastanadia Datu Sompie	Optimization and characterization of Chitin-Collagen based wound dressing functionalized withsilver Nanoparticles (AgNPs)
13:10	**TP11**	Sara Ghazy	Development of novel opioid peptidomimetics through Tyrosine modifications in endomorphins
	Discussion		
13:40	**Lunch**		

Session 3 Chemical sustainability and circular economy

Chairperson: *Alessandra Tolomelli*

15:30	**Keynote 2**	Jacopo Monaldi (ECHA)	Sustainability and implementation of European chemical regulation
16:10	**TP12**	Elizabeth Alvarez Prez	Rare earth magnet dynamics: A material flow analysis of rare earth permanent magnets in electric vehicle traction motors for passenger cars in the EU-27
16:20	**TP13**	Getachew Gebrehiwet	Carbon Capture and Utilization (CCU) for production of renewable chemicals: preparation and test of novel biochar-based material for homoacetogenic reactor
16:30	**TP14**	David Moses Kolade	Enhancing phosphate recovery: magnesium oxide-modified biochar for wastewater treatment
16:40	**TP15**	Prince Ebo-Donkor	Solar/Cl_2 process for wastewater remediation: characterization and performance
16:50	*Discussion*		
17:10	***Closing of day 1***		

Tuesday, July 9

Session 4 **Chemical Regulations and Environmental Law**

Chairperson: *Carme Gonzalez*

09:30	**Keynote 3**	Serenella Sala (JRC)	Safe and sustainable by design chemicals and materials: an integrated framework to steer innovation
10:10	**TP16**	Abdul Rahman Miraj	Evaluating REACH 2.0 in the context of the chemical strategy for sustainability within the EU Green Deal agenda
10:20	**TP17**	Ana Diges	Environmental sustainability and indigenous knowledge: testing rights of nature before United States courts
10:30	*Discussion*		

Session 5 **Nanomaterials and Sensors**

Chairperson: *Santiago Esplugas*

10:10	**TP18**	Jalal Ahmad	Synthesis and photophysical characterization of novel heterometallic Gold(I)-Copper(I) complexes
10:20	**TP19**	Mariam Abramishvili	Effects of leptin-derived peptides on β-amyloid folding patterns and aggregation inhibition
10:30	**TP20**	Marlen Mustafin	Safe and Sustainable by Design hybrid nano-structures
10:40	*Discussion*		
11:00	**Coffee break** *Poster Session*		
11:20	**TP21**	Gideon Asew Boafo	Two-dimensional transition metal dichalcogenides for gas sensing applications
11:30	**TP22**	Sharon Otieno	Extended triphenylene-based metal-organic frameworks for sustainable catalysis
11:40	*Discussion*		

Session 6 **Innovation in Food**

Chairperson: *Daniel Sainz*

12:00	**Keynote 4**	Coral Verge (CEPSA)	Trends in Products Stewardship : from Chemical Safety to Chemical Sustainability
12:40	**TP23**	Adrine Elisabeth Ganimian Tcharkhetian	Towards the generation of full AMPK model combining experimental and computational techniques
12:50	**TP24**	Aysha Siddika	Total polyphenols in commercial foods: quantification and computational analysis as na integral part of the mediterranean diet framework
13:00	**TP25**	Sultana Chowdhury	Formation of pullulan-pectin hybrid gels for the obtaining of pullulan beads by dripping method. Rheological study and evaluation as active ingredient release systems
13:10	*Discussion*		
13:20	**Lunch**		

Session 7 **Chemical Sustainability**

Chairperson: *Emilio Tagliavini*

15:30	**Keynote 5**	Guillem Domènech (University of Barcelona)	Solid state gas sensors: from materials to devices
16:10	**Keynote 6**	Anna Bielinsky (University of Gdansk)	The PARC project: Partnership for the Assessment of Risks from Chemicals
17:20	**Awards Session**		
18:00	***Closing session***		

Research Theses Presentation Abstracts

(Oral and Poster)

Lycopene extraction from tomato waste using sustainable solvents

Bryan Leonardo Morales Espino[(a),(b)], Cecilia Sepe[(b)], Vanessa Spadavecchia[(b)], Chiara Samorí[(b)], Paola Galleti[(b)]

[(a)]Erasmus Mundus Joint Master Degrees (EMJMD) in MSc. Chemical Innovation and Regulation (ChIR), [(b)]Dipartimento di Chimica "Giacomo Ciamician" , Ravenna Campus, University of Bologna, Via Sant' Alberto 163, 48123 Ravenna, Italy.

The global production of fresh tomatoes exceeds 180 million tonnes annually, with around 40 million tonnes dedicated to processing, generating significant byproducts, mainly skins, seeds, and pulp residues.[1] Lycopene, which gives tomatoes their red color, has potent antioxidant properties and various health benefits, including cancer prevention and cardiovascular protection.[2] Conventional lycopene extraction methods often use toxic organic solvents. Sustainable alternatives like Deep Eutectic Solvents (DES) offer comparable efficiencies and are environmentally friendly. In this study, lycopene extraction from tomato peel waste using traditional and alternative solvents, including lipophilic DES, were investigated. The highest lycopene yield of 0.11 mg/g (considered as 100% benchmark) was achieved using 2-MeTHF. DES prepared with Menthol: Thymol at different molar ratios achieved extraction efficiencies up to 112%. Optimal conditions included 90ºC, biomass ratio 1:10 (m/v), no light exposure, and constant stirring for 2 hours. DES methods proved more efficient than traditional and alternative solvents and offer an eco-friendly extraction approach.

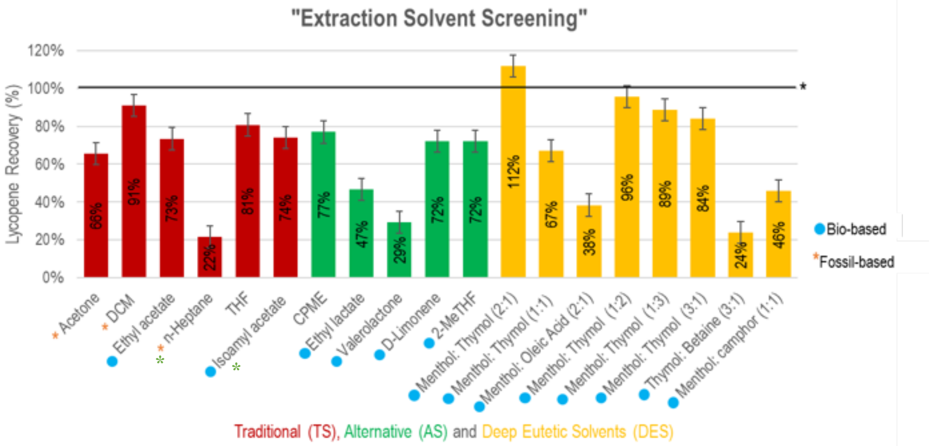

Figure 1. Extraction Solvent Screening using Traditional, Alternative, and Deep Eutectic Solvents. *****A 100% Lycopene yield was obtained through solid-liquid extraction using 2-MeTHF until the solution residue became colorless.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References:

[1] World Processing Tomato Council (WPTC). (2024) Production of Fresh Tomatoes. Retrieved 11 June 2024, from https://www.wptc.to/

[2] Eslami, E., Carpentieri, S., Pataro, G., & Ferrari, G. (2022). A Comprehensive Overview of Tomato Processing By-Product Valorization by Conventional Methods versus Emerging Technologies. Foods, 12(1), 166. https://doi.org/10.3390/foods12010166.

Development of 4th generation batteries quality control in the lamination process

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(a)*Department of Chemistry "G.Ciamician", Bologna University;* (b)*Testing Department, Manz Italy*

Battery industry is constantly innovating and developing new batteries generation. Nowadays, the 4th generation batteries are in a very advanced stage. These batteries are called solid batteries because the electrolyte filling is substituted by solid separators with the electrolyte.[1]

The presented thesis studies the adaptation of the 4th generation batteries in the lamination process. To do so, it will be checked the lamination conditions, developed a quality control for this lamination process, and evaluate the viability and cycle time to insert the quality control check process in a lamination machine.

The lamination of the 4th generation batteries has been viable only under limited conditions. Moreover, uncommon methods have been used to achieve a minimal adhesion. For example, paper has been added to the lamination process to achieve the adhesion and it has been studied that with its incorporation the battery does not lose weight during the process.

Later, AC Impedance measurements and the ionic conductivity have been measured to non-laminated samples and laminated samples under different lamination parameters. The AC Impedance measured with a more potent instrument which also allows to calculate the ionic conductivity shows a good differentiation between the non-laminated samples and the different laminated samples in both measurements. On the other hand, the AC Impedance has been measured with a simpler instrument which only shows 5 points per spectra, and it does not allow to calculate the ionic conductivity. With this instrument it has also been possible to differentiate between all the lamination conditions and non-laminated samples.

Therefore, it has been found a test which allows to differentiate between different lamination conditions and could work as a quality control technique. This test can be done with the first instrument resulting with a better quality control, but slower or a faster and simpler with the second instrument.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References:

[1] T. Kim, W. Song; *J. Mater. Chem. A* **2019**, 7(7), 2942-2964.

Redesigning polyurethane cavity filling acoustic foam for increased safety and sustainability

Breno Savazini Leone(a), Fabrizio Passarini(a), Luca Ciacci(a), Daniele Cespi(a), Vanni Parenti(b), Lorenzo Musiani(b)

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This study, conducted in partnership with Dow Italia, aims to redesign a polyurethane material used as Cavity Filling Acoustic Foam in automotive industry (Figure 1) to enhance its safety and sustainability. Polyurethane foams are formed by the reaction between polyol and isocyanate, leading to volume expansion.[1] Plasticizers are added in this process to improve the processability and properties of the product.[2] The study focuses on the substitution of the current plasticizer due to its potential release and listing on the SIN List ("Substitute It Now!" List). Safer and more sustainable plasticizer alternatives were evaluated by applying the Safe and Sustainable by Design (SSbD) framework.

Alternative plasticizers were identified and screened, leading to two candidates selected for technical evaluation. The safety assessment showed that these alternatives meet the SSbD Step 1 hazard profile requirements. However, the environmental sustainability assessment revealed that the renewable-based alternative had a slightly higher Product Carbon Footprint (PCF).

Technical performance tests demonstrated that Alternative 1 had satisfactory sound absorption and adhesion properties but initially failed the water absorption test. Adjustments in foaming parameters were made, and the water absorption of Alternative 1 is under reassessment together with Alternative 2.

The study suggests that while the SSbD tool is effective for guiding product assessments, its complexity and data requirements are very challenging. This study highlights the need for more comprehensive data and tailored methodologies to ensure accurate and effective sustainability evaluations in polymer product design, preventing misdirection in innovation decisions.

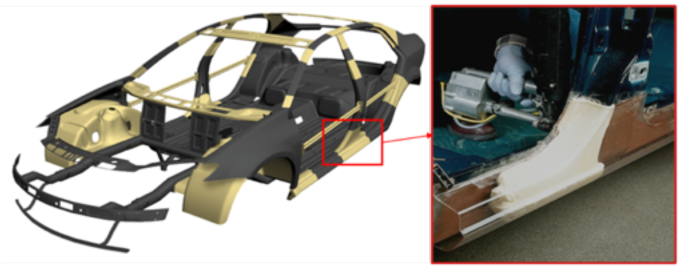


Figure 1. Polyurethane Cavity Filling Acoustic Foam: demonstration of application areas within car cavities.

Acknowledgments: We acknowledge Dow Italia for their invaluable partnership and provision of necessary resources and capabilities for the development of this case study. We also extend our gratitude to the University of Bologna and Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD, for supporting this research project.

References:

[1] N. V. Gama, A. Ferreira, A. Barros-Timmons; Materials 2018, 11, DOI 10.3390/ma11101841. [2] P. H. Daniels; Journal of Vinyl and Additive Technology, 2009, 15, 219–223.

TP 4 and Poster 4

Development of green chitin-based materials for thermal insulation and packaging applications

Bositkhon Akhmedov, Devis Montroni, Angelica Mucaria

Department of Chemistry "Giacomo Ciamician", University of Bologna.

A simple and environmentally friendly method was developed to create a porous material entirely from β-chitin, avoiding the use of high pressures and toxic solvents.

Chitin is a natural polymer insoluble in water, consisting of N-acetyl-D-glucosamine linked by β-1,4-glycosidic bonds, and exists in three polymorphs: α-chitin, β-chitin, and ɣ-chitin. It is the second most abundant polymeric polysaccharide after cellulose, with an annual production of 16.6 million metric tons in 2019 and exhibits good biocompatibility and degradability.[1,2]

In this study, we focused on β-chitin, where the polymer chains are oriented parallel to each other. This alignment results in a structure that is more accessible to solvents than the other polymorphs, making it easier to process.[3] Thermal conductivity testing of the optimized chitin foam revealed a thermal conductivity factor in a range of 0.028-0.030 W/(m·K), which is on par with standard insulating materials that have thermal conductivity values below 0.06 W/(m·K).[4] Thermogravimetric analysis indicated that the chitin-based material is thermally stable up to 200 ºC. Mechanical compression tests suggest that this material could also be suitable for packaging applications.

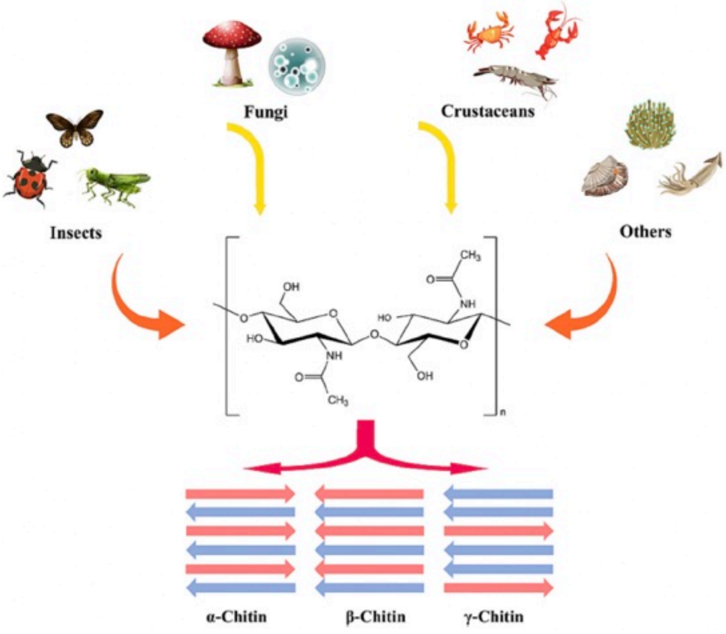


Figure 1. Chemical structure of chitin and its polymorphs.[1]

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References:

[1] Jiran Lv, Xiaohui; *Carbohydrate Polymers* **2023**, vol, 299. [2] Amiri H, Aghbashlo M; *Nature Food* **2022**, vol, 3. [3] Yang, F. C., Peters, R. D; *Soft Matter* **2014**, *10*,5541-5549.
[4] A. Kylili, P.A. Fokaides; *Cost effective energy efficient building retrofitting* **2017,** p, 23-55.

Cyclopalladation of α-amino acid Schiff bases and their applications in Suzuki reactions

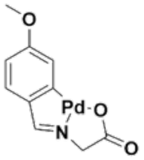
Alex Kamande, Joan Albert, Daniel Sainz

Inorganic and Organic Chemistry Department, Inorganic Section, Barcelona University, Martí i Franquès 1-11, 08028 Barcelona (Spain)

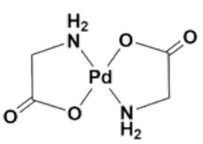
The synthesis of cyclopalladated compounds is interesting due to their potential applications in medicine and as precatalysts in C-C or C-heteroatom coupling reactions.[1] α-amino acid imine palladacycles are prepared via a 4-step procedure[2] that is time consuming and results to chemical wastage. Our research group has reported a one pot procedure for the synthesis of imine palladacycles.[3] However, this procedure is yet to be studied for imine palladacycles derived from α-amino acids.

Reacting equimolar amounts of $Pd(OAc)_2$, glycine and p-anisaldehyde in HOAc, small amounts of a tridentate imine palladacycle **1A** were detected in solution by ^1H NMR, with the main product being the bis(glycinato)palladium(II) complex **1B**. To prevent the coordination of oxygen to Pd which lead to the formation of bis(glycinato)palladium(II) complex, the use of glycine esters was considered. Reacting equimolar amounts of $Pd(OAc)_2$, glycine ethyl ester hydrochloride, p-anisaldehyde and KCl in HOAc produced a bidentate palladacycle **2A** with yields varying from 23 – 51 %, depending on the reaction conditions. Splitting reaction of compound **2A** with equimolar amounts of $[NiCl_2(PPh_3)_2]$ in acetone at room temperature acquired the mononuclear compound **3A** whereas, using equimolar amounts of 2,4,6-trimethylpyridine, the mononuclear compound **3B** was obtained. Furthermore, coordination compound **4A** was synthesized by reacting in HOAc glycine ethyl ester hydrochloride with $Pd(OAc)_2$ in molar ratio 2:1. All compounds were characterized by NMR, FTIR, ESI mass spectrometry and elemental analysis. In addition, the crystal structure of compound **4A** has been determined by single X-ray diffraction analysis. Compounds **1B**, **2A**, **3A**, **3B**, and **4A** are being tested as precatalysts for Suzuki C-C cross coupling reactions between phenyl boronic acid and bromo phenyl substrates.

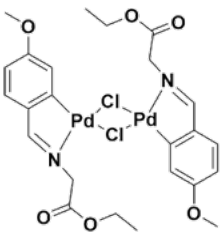
1A



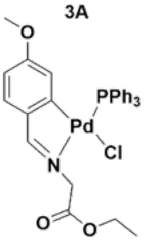
1B



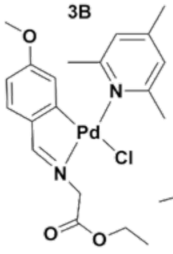
2A



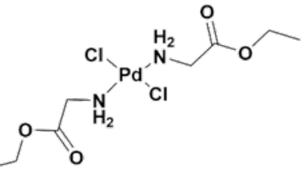
3A



3B



4A



Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References:

[1] Dupont J, Consorti CS, Spencer J. The Potential of Palladacycles: More Than Just Precatalysts. Chem Rev. **2005**;105(6):2527-2572. doi:10.1021/cr030681r. [2] Albert J, Crespo M, Granell J, et al. Cyclopalladation of Schiff Bases from Methyl Esters of α-Amino Acids. Unexpected Activation of the O−Me Bond with Formation of a Bianionic Tridentate Metallacycle. Organometallics. **2010**;29(1):214-225. doi:10.1021/om9009153. [3] Albert J, Barreira A, Granell J, et al. Three Component One Pot Synthesis of Endo Cyclopalladated Imines. In: XL Meeting of the Specialized Group on Organometallic Chemistry. Specialized Group on Organometallic Chemistry; **2022**:01-01.

Synthesis of magnetic hybrid Core@Shell nanomaterials: Fe_3O_4 nanoparticles coated with spin crossover polymer

Ayoub Antar, Marta Estrader

Department of Inorganic and Organic Chemistry, University of Barcelona, Barcelona Spain

The reversible transition between high-spin (HS) and low-spin (LS) states in some transition metal complexes is known as the Spin Cross-Over (SCO) phenomenon. Temperature and light intensity are two examples of external inputs that affect this process. Fe(Htrz)2(trz) SCO complex can be applied to iron oxide (Fe_3O_4) nanopartiles in a core@shell structure to achieve this effect. The complex can be heated using the iron core to induce the HS state, which qualifies the material for a number of technological uses, such as ON/OFF systems and data storage. This paper shows the utilization of iron oxide nanoparticles as a more economical and effective substitute for the gold nanoparticles utilized in previous research projects. The nanoparticles were synthesized using the solvothermal method, and the SCO complex was grown on their surface after transferring them from the organic medium to water. TEM-EELS analysis confirmed the core@shell structure, showing a clear iron core enclosed by an outer layer that contains iron, nitrogen, and oxygen.

Acknowledgments: this master thesis have been funded by Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References:

[1] H. Gavilán, G. M. R. Rizzo, N. Silvestri, B. T. Mai, and T. Pellegrino, "Scale-up approach for the preparation of magnetic ferrite nanocubes and other shapes with benchmark performance for magnetic hyperthermia applications," Nature Protocols, vol. 18, no. 3. Springer Nature, pp. 783–809, Mar. 01, 2023. doi: 10.1038/s41596-022-00779-3. [2] E. Coronado, J. R. Galán-Mascarós, M. Monrabal-Capilla, J. García-Martínez, and P. Pardo-Ibáñez, "Bistable Spin-Crossover Nanoparticles Showing Magnetic Thermal Hysteresis near Room Temperature," Advanced Materials, vol. 19, no. 10, pp. 1359–1361, May 2007, doi: 10.1002/ADMA.200700559. [3] R. Torres-Cavanillas, R. Sanchis-Gual, J. Dugay, M. Coronado-Puchau, M. Giménez-Marqués, and E. Coronado, "Design of Bistable Gold@Spin-Crossover Core–Shell Nanoparticles Showing Large Electrical Responses for the Spin Switching," Advanced Materials, vol. 31, no. 27, Jul. 2019, doi: 10.1002/adma.201900039. [4] R. Torres-Cavanillas, R. Sanchis-Gual, J. Dugay, M. Coronado-Puchau, M. Giménez-Marqués, and E. Coronado, "Design of Bistable Gold@Spin-Crossover Core–Shell Nanoparticles Showing Large Electrical Responses for the Spin Switching," Advanced Materials, vol. 31, no. 27, Jul. 2019, doi: 10.1002/adma.201900039.

TP 7 and Poster 7

New catalyst for CO_2 conversion via the Reverse Water-Gas Shift (RWGS) reaction

Sunday Perfect Peace[(a)], Narcis Homs[(a)(b)], Prof. Pilar Ramirez de la Piscina[(a)]

[(a)]Department de Quimica Inorganica i Organica, Seccio de Quimica Inorganica, Universitat de Barcelona, Martí i Franquès 1, 08028, Barcelona, Spain, [(b)]Department of Inorganic and Organic Chemistry and Institute of Nanoscience and Nanotechnology, University of Barcelona, Spain.

Efforts have been made to develop an efficient catalyst for sustainable CO_2 conversion into useful products via the reverse water gas-shift process (RWGS). Transition metal carbides are found to have high activity, selectivity, stability and resistance to sintering in the RWGS process and most importantly they are low-cost materials which make them attractive and suitable alternatives for noble metal catalyst.[1,2].

In this research, chromium and molybdenum MAX Phases (Cr_2AlC, Mo_3Al_2C), MXenes (DS_i-Cr_2CTx, DS_i-Mo_3CTx) and carbides (Cr_3C_2, Mo_2C) were employed to develop CeO_2-ZrO_2 supported and, Ni- and Co-modified composite catalyst for application in the RWGS process. Synthesis of MXene was done through MAX Phase etching utilizing a mild $FeCl_3.6H_2O$ + Tartaric acid exfoliation technique, followed by delamination in DMSO. Incipient wetness impregnation was employed to incorporate the Ni and Co metals into the support. ultrasonic probe technique was employed to form homogeneous mixture of the MAX Phases, MXenes, carbides and the support material. All prepared catalysts were characterized by XRD, SEM-EDS, and TPR before catalytic test in RWGS process up to 600 °C maximum temperature with reactant gas mixture of CO_2/H_2 =1/3 molar ratio, and gas hourly space velocity of 3000 h^{-1}.

Result of the RWGS test revealed that CO_2 conversion increased with increased temperature. Co/CZ/DS_1-Cr_2CTx catalyst had CO_2 conversion of 92.5% and CO selectivity of 96.7% at 400 °C. Methane formation was highest in Co/CZ catalyst at 400 °C. Addition of MAX phase, Mxene and carbide helped reduce CH_4 formation. The ability of these catalysts to deliver high conversion and selectivity at lower temperature is pivotal to large scale RWGS process, as energy demands have been a significant limitation.

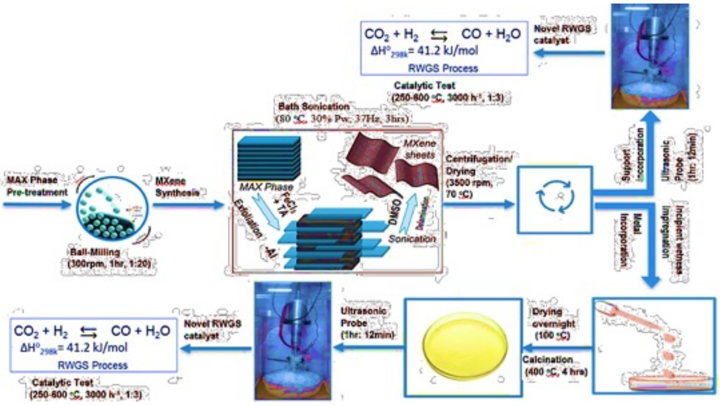


Figure 1. Graphical Abstract

Acknowledgements: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References:

[1] D. Dolz et al., "Understanding the Reverse Water Gas Shift Reaction over Mo_2C MXene Catalyst: A Holistic Computational Analysis," ChemCatChem, p. e202400122, 2024, doi: 10.1002/CCTC.202400122.
[2] K. P. Reddy et al., "Molybdenum carbide catalyst for the reduction of CO2 to CO: surface science aspects by NAPPES and catalysis studies," Dalton Transactions, vol. 48, no. 32, pp. 12199–12209, Aug. 2019, doi: 10.1039/C9DT01774G.

Study of MAX phases and 2D-derived materials for CO_2 conversion through the reverse water gas shift reaction

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Global warming and climate change have been the bane of the world and pose a great threat to the development, security, and existence of mankind. Carbon dioxide (CO_2) has been proven to contribute to global warming and climate change significantly. Utilizing CO_2 through chemical recycling and conversion into usable products is one of the most promising options for regulating the global carbon balance and mitigating global warming.[1] The reverse water gas shift pathway reacts CO_2 with H_2 to produce CO and H_2O (syngas) which can be used in Fischer-Trophsch synthesis, or for methanol production.[1]

MAX Phases and 2D-derived Mxene materials have recently sparked interest in materials research. MXenes have proven very promising and useful in applications as catalytic materials and electrode materials for energy storage due to enhanced metal−support interactions.[2,3]

In this work, we carried out the synthesis of MAX phases based on Mo and V with Ga and Zn as 'A-group' elements employing solid-state reactions. Synthesis of 2D MXene derivatives from the as-prepared Mo_2Ga_2C and Va_2GaC MAX precursors using the UV-induced selective etching method was carried out. The etching of Al from commercial Mo_3Al_2C by the Lewis acid molten salt method has also been explored. These etching techniques avoid the use of fluorine-based etchants thus making the process much greener and safer.

Catalysts were prepared by incorporating metals such as Cu and Ni using a one-pot synthesis approach and incipient wetness impregnation method. Materials were characterized by employing various characterization techniques (XRD, SEM-EDS, H_2-TPR). The catalytic behavior was also studied in the reverse water gas shift reaction (RWGS) at 200-600°C, CO_2:H_2 =1:3 (molar ratio); P= 1 atm; GHSV =3000 h^{-1}.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Microwave assisted synthesis of heterometallic lanthanoid 2D metal-organic frameworks

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Metal-Organic Frameworks (MOFs) are highly porous crystalline materials composed of metal ions coordinated to organic ligands, known for their exceptional thermal stability, large surface area, and tunable properties, making them ideal for applications in gas storage, catalysis, drug delivery and sensing.[1,2] Despite their potential, traditional synthesis methods, such as solvothermal and hydrothermal processes, are time-consuming and often result in low yields and poor phase purity. This study explores microwave-assisted synthesis to produce heterometallic lanthanoid 2D MOFs, which led to the discovery of novel MOFs with the general formula $[(Ln_xLn_{1-x})_4(PhCOO)_9(MeCOO)_3(MeOH)_3(H_2O)]\cdot MeOH\cdot MeCN$, the study include both homonuclear (Ln=La,) and heterometallic compounds ([LaEu]), ([LaGd]) with varying lanthanide molar ratios.

The microwave-assisted method offers rapid and uniform heating, significantly reducing synthesis times from hours to minutes while enhancing the quality and yield of the MOFs. Characterization of the synthesized MOFs revealed good thermal stability and significant gas sorption properties, including promising sensing capabilities and potential for application in quantum qubits.[3]

The implications of this research are significant, indicating that microwave-assisted synthesis can produce high-quality MOFs with enhanced properties suitable for various applications. This study has opened avenues for testing the potential applications of the new MOFs, exploring new heterometallic combinations, and assessing its real-world applicability in various fields.

Acknowledgements: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Optimization and characterization of chitin-collagen based wound dressing functionalized with silver nanoparticles (AgNPs)

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Efficient wound healing for burn injuries remains a challenge due to excessive exudate and high infection risk. Chitin-collagen scaffolds, due to their combination of biocompatibility and mechanical strength, serve as a promising solution to this challenge as it can function as wound dressing and aid the wound healing process by promoting tissue regeneration and reducing infection.[1,2] Previous studies in our research group identified the 75:25 chitin-to-collagen ratio as yielding the most promising results, leading to optimization of scaffold preparation using this ratio.[3]

Optimization revealed that using commercial chitin instead of the chitin purified by our team made the process more practical without inducing changes in the final material. Additionally, employing a -20 °C freezing process instead of liquid nitrogen reduced energy consumption and improved the material's mechanical resistance and stability. This study also explored the use of crosslinkers, such as glutaraldehyde, which resulted in scaffolds with enhanced properties. Characterization with a mechanical compression test showed that the modified scaffolds with 0.5% and 1% glutaraldehyde exhibited increased toughness. This was indicated by a Young's modulus value up to 130 Pa and densification occurring at over 86% deformation and at about 26 kPa of stress, compared to the control scaffold with a Young's modulus of 55 Pa and densification occurring at over 77% deformation and at about 6 kPa of stress.

Successively, the incorporation of silver nanoparticles (AgNPs) into the wound dressings was exploited to introduce antimicrobial properties.[4] The scaffold was functionalized with AgNPs, testing two sizes of AgNPs 10 nm and 17 nm. Functionalization of the AgNPs into the wound dressing scaffold was performed in two ways: adding the AgNPs during the scaffold synthesis (>95% integration of AgNPs) and adsorption on the finished scaffold (>90% integration of AgNPs).

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Development of novel opioid peptidomimetics through Tyrosine modifications in endomorphins

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The opioid crisis remains a significant global health concern, with approximately 85,000 individuals in Europe seeking specialized drug treatment programs annually due to opioid use.[1] While opioids effectively manage severe pain, they also induce serious adverse effects such as addiction, dependence, respiratory depression, criminal behavior, and tolerance. Endogenous opioid peptides, released in the CNS, offer powerful pain-relieving effects and are considered safer alternatives to traditional opioids. However, their clinical use is limited due to challenges like low stability and poor bioavailability. These issues are being addressed through peptidomimetic modifications, which involve altering the structure of the opioid peptides to optimize their interaction with opioid receptors (MORs, KORs and DORs), thereby enhancing therapeutic efficacy while reducing adverse effects.[2] Owing to their potent analgesic effects, therapeutic effectiveness of Endomorphins-1 (EM1) – a class of opioid peptides - has been extensively studied through modifications at the Tyr position using a novel method that introduces urea groups via reactions with isocyanates, as illustrated in Figure 1. The results obtained thus far are notably promising and intriguing. Given the high selectivity of EM1 for MORs, some modified molecules demonstrated high binding affinity for MORs, others shifted their affinity towards KORs and DORs, and some entirely lost their binding affinity. These findings highlight an opportunity to advance EM1 in drug discovery and expand its therapeutic applications in pain management, marking a significant step toward developing more effective opioid peptide therapeutics.

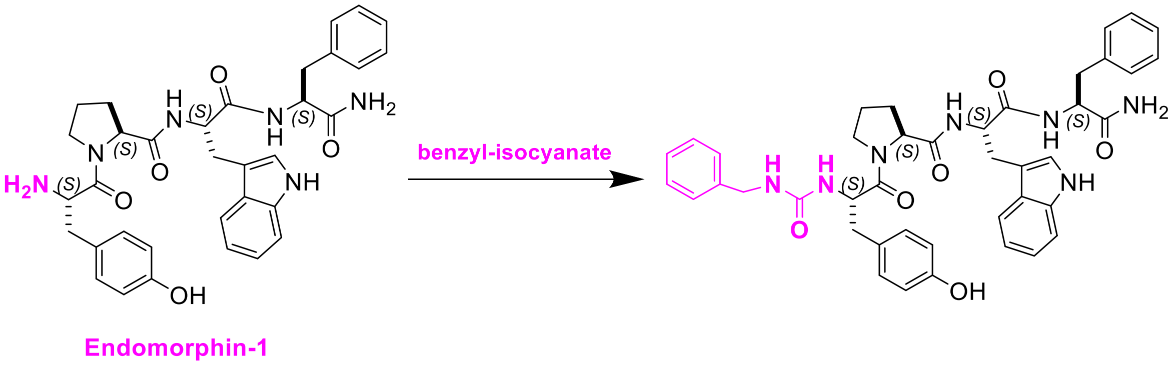

Figure 1. Illustration of the Tyr modification of EM-1.

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Rare earth magnet dynamics: A material flow analysis of rare earth permanent magnets in electric vehicle traction motors for passenger cars in the EU-27

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The transition towards clean energy and the "Beginning of the End" of the Fossil Fuel Era as called for by COP 28, is driving the rise of technologies such as electric vehicles (EVs). In this context, it is crucial to ensure the availability of critical materials for their manufacture. One example is rare earth permanent magnets (REPM), such as neodymium-iron-boron (NdFeB), used in EV traction motors. Neodymium and dysprosium, components of these magnets, have been identified as critical materials with supply chain risks.[1] To mitigate these risks, circular economy strategies have been proposed.

This study analyzes the use of REPM (NdFeB) in the European Union-27. It focuses on the traction motors of passenger cars (N1-M1 categories), estimating the flows of these materials. Additionally, a dynamic model is developed to predict the flows at the end of life (EoL) of EVs containing REPM.[2] The amount of NdFeB magnets potentially recoverable from EVs at the end of their life is evaluated and its importance as a secondary source of rare earths is assessed in relation to the estimated demand for this type of electric vehicle in the EU-27.

The results show that if a collection rate of 100% and a recycling rate of 98% are achieved, approximately 4.5% of the demand for NdFeB magnets for EVs in 2040 could be met. While the projected amount of secondary REPM is smaller compared to the total demand for EVs, its recovery could cover a significant portion of future demand if its life cycles can be circularized.

The stocks and flows estimated in this study are relevant for informing public policies that support the development of secondary materials markets. These policies should drive higher collection rates and greater recycling efficiency.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Carbon Capture and Utilization (CCU) for production of renewable chemicals: preparation and test of novel biochar-based material for homoacetogenic reactor

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One promising strategy for the long-term, renewable use of resources is the biological conversion of hydrogen and carbon dioxide into useful chemicals using mixed microbial cultures (MMC) [1][2]. The present study introduces a novel biochar-polystyrene (biochar-PS) composite sparger in a char-based biofilm sparger reactor (CBSR) to optimize volatile fatty acid (VFA) production. Two types of spargers were designed, installed, and tested (Closed-Top and Open-Top), to resolve previous limitations[1] and illustrate the biochar PS sparger's scalability.[2] The sparger in both reactors comprised of a 4:3 biochar to polystyrene mass ratio. The CBSR systems were assessed under various conditions, such as dilution rates, operational modes, carbonate content, and operating volumes. In this study, a thorough evaluation of sparger performance was conducted for 4 months. The sparger was upgraded with a distinctive design to improve biofilm formation and mass transfer. The system has attained a volumetric productivity of 19 $gCODL^{-1}D^{-1}$, a maximum VFA concentration of 60.55 gCOD/L at 35°C, a pH of 6.9, and a dilution rate 0.1 D^{-1}. The Closed-top and open-top systems were both effective; however, the open-top system's improved gas-liquid-solid interaction resulted in a more efficient biofilm formation and mass transfer process. The increased bubbling activity in the system with open-top sparger facilitates the squeezing of produced VFA, reducing inhibition and facilitating greater microbial activity and gas transfer. These results illustrate the feasibility and scalability of the biochar-PS sparger design in improving VFA production. The study makes a substantial contribution to circular economy, and power to X by thoroughly examining sparger performance under various operational conditions and demonstrating the feasibility of biochar-PS composites in scalable bioreactor applications. The implications of this study are extensive, indicating that biochar-PS spargers could revolutionize fermentation processes with suitable design modifications.

The sparger design should be further optimized, and its applications in other biofilm mediated fermentation systems should be the primary focus of future research.

Keywords: biochar-polystyrene sparger, CBSR, volatile fatty acids, gas-liquid-solid mass transfer, biofilm formation, scalable bioreactors, fermentation optimization, power to X.

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Enhancing phosphate recovery: magnesium oxide-modified biochar for wastewater treatment

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As industry and agriculture rapidly advance, the annual discharge of phosphorus-rich domestic, industrial, and agricultural wastewater is rising. While phosphorus is essential for life and agriculture, its overuse and environmental release lead to problems like eutrophication. Moreover, heavily exploited phosphate rock deposits are finite and nonrenewable. Thus, there is growing interest in finding solutions to the challenges posed by limited supply, increasing demand, and the environmental impact of phosphorus.[1]

Various methods are employed to recover phosphorus from wastewater, including biological processes, chemical precipitation, electrolysis, and adsorption. Among these, biochar adsorption has gained attention for its significant environmental and economic benefits. While biochar's negative surface charge initially limits its affinity for phosphate anions, its adsorption capacity can be enhanced through structural modification.[2,3]

Magnesium oxide-modified biochar (MgO-B) has proven to be a highly effective adsorbent with excellent phosphate affinity.[3] This study evaluates a method for producing biochar loaded with MgO to improve phosphate adsorption. Biomass, shredded to desired sizes, was treated with various $Mg(NO_3)_2$ ratios (10-30:100) at room temperature, stirred for 24 hours, then dried and pyrolyzed at 10°C/min up to 900°C in a tubular furnace for up to 3 hours under nitrogen flow. A face central composite design from a response surface methodology was used to optimize the effects of biochar pyrolysis temperature, time, and $Mg(NO_3)_2$ concentration on the adsorption capacity. Adsorption experiments were conducted, and residual phosphates were analyzed calorimetrically using the molybdenum blue method via UV-Vis spectrophotometry. MgO-B demonstrated good phosphorus adsorption (185.0713 mg/g), outperforming pristine biochar (6.4477 mg/g) and commercial activated carbon (4.7749 mg/g). It was determined that the only factor affecting the adsorption capacity was the concentration of $Mg(NO_3)_2$. The results exhibit a trade-off between yield and adsorption capacity, as increasing the salt concentration always leads to a decrease in the biochar yield but significantly increases the adsorption capacity. These findings suggest that this technology is a promising alternative for phosphorus recovery from wastewater and supports further research into using these materials directly as fertilizers. Further investigation is ongoing to characterize the biochar products using SEM-EDS, FTIR, TGA, and BET analyses and to study the adsorption isotherm model and kinetics.

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Solar/Cl_2 process for wastewater remediation: characterization and performance.

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The declining quality of global freshwater supplies due to the presence of micropollutants (MPs) in water poses a severe threat to public health. This group of pollutants includes persistent organic pollutants (POPs), pharmaceuticals, pesticides, and personal care products. To compensate for the growing global demand for freshwater, water reclamation (reuse) has been touted as a brilliant idea to achieve this feat.[1,2] Considering that treatment technologies currently implemented in wastewater treatment plants (WWTPs) are not effective in eliminating MPs, this poses an impediment towards achieving water reclamation goals.

To achieve a significant attenuation of the MPs in the treatment plants and to reduce the associated risks, this study proposes an innovative Advanced Oxidation Process (AOP) based on solar (sunlight) and chlorine combined with a probe compound-based kinetic model developed for a generalized prediction of MPs abatement in various water matrices. Employing solar radiation in UV-based systems forms an attractive option with a significant reduction in operational costs. A lab-scale experiment in a solar simulation chamber (Atlas SUNTEST CPS+) was conducted to study the remediation of probe compounds and evaluate the performance of the process.

Results indicated that naproxen is the easiest to eliminate with a removal efficiency of 55% at 5ppm of chlorine and a complete removal at 10 ppm to 50 ppm of chlorine. Also, primidone was the least removed with removal efficiencies of just above 5% removal at 5ppm of chlorine and a maximum removal of about 35% achieved at 50ppm of chlorine. Additionally, it was observed that photolysis has trivial effects on the degradation process of most of the compounds, except for dimetridazole (about 25% removal) and naproxen (about 10% removal).

The results show that by measuring the depletion of probe compounds spiked in the wastewater matrix, the exposures of main reactive chlorine species including chlorine radicals (Cl•), dichloride radicals (Cl_2^{-}•) and chlorine oxide radicals (ClO•), and hydroxyl radicals (•OH) during the solar/chlorine process could be calculated using the kinetic model. Based on the determined exposures, the abatement efficiencies of various MPs in different wastewater matrices could generally be predicted with acceptable accuracy by the model without prior water-specific calibration making the probe-based kinetic model a useful tool to guide practical water and wastewater treatment for MPs abatement.

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Evaluating REACH 2.0 in the context of the chemical strategy for sustainability within the EU Green Deal Agenda

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The main goal of chemical regulation is to protect human health and the environment from chemical risks, adapting to new scientific evidence as it emerges. In the European Union, the key regulations REACH 1907/2006 and CLP 1272/2008 play a crucial role. REACH 2.0 addresses critical updates and initiatives under the Chemical Strategy for Sustainability (CSS), aiming to achieve climate neutrality by 2050. Key updates as of June 2024:

REACH Registration of Polymers, 1-10 Low Tonnage Band, and Nanoforms. Information requirements for safety data sheets, ecotoxicological data, and exposure scenarios. Updates in Registration Dossier Preparation in IUCLID 6. Addition of Mixture Assessment Factor (MAF) in Evaluation Reforms to account for the combined effect of chemicals present in the environment. Introduction of New Approach Methods (NAMs) such as Read-Across, QSAR, and Data Waiving tools to support non-animal testing, including the use of in vitro (test tube or cell culture) experiments to predict how a substance will behave in a living organism (in vivo).

Restriction of substances using the Generic Risk Approach (GRA) that regulates multiple substances together based on shared risks, characteristics, and similar properties. Ban on PFAS; restrictions on bisphenols, phthalates, and CMR, ED, PBT, and vPvB substances. Essential use is possible but only for a specific period with a proposed plan for alternatives. Authorization specifically applies to SVHCs and involves granting permission for essential use under controlled conditions, ensuring risks are adequately managed. Addition of Derived Minimal Effect Levels (DMELs) for non-threshold substances, meaning any exposure carries some risk.

The "One Substance, One Assessment" approach is a central data platform for unified access under EU legislation, involving collaboration between ECHA, EMA, EEA, EFSA, and national authorities. This approach includes reallocating work to EU agencies, improving access to chemical data, and modernizing the ECHA (COM (2023) 779).

Economic Analysis by Ricardo Plc Faster, 5 Years Implementation

Scenario	Turnover Loss €B	GVA Loss €B	Regulatory Burd. €B	Job Losses
Add. in CLP	67.0	57.0	0.518	106,000
Export Ban	9.5	8.3	0.530	15,700
MAF	0.7 - 5.3	0.2 - 1.4	0.0	500 - 5,600
Polymer Reg.	0.58	3.2	1.600	1,500

Overall, the results of the study suggest that the updated regulations under REACH 2.0 and CLP will impose economic and administrative burdens on chemical companies in the EU. The export ban on certain chemicals will significantly impact EU exporters' ability to access the global market.

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Environmental sustainability and indigenous knowledge: testing rights of nature before United States courts

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A pioneering RoN case used to challenge the construction of an oil pipeline in the United States has exposed the inadequacies of Western environmental regulatory models. Set in Minnesota, this case involved the crossing of indigenous ceded lands and reservations, threatening the culturally significant wild rice (Manoomin).[1] The 2018 Rights of Manoomin tribal law was employed to contest the Minnesota Department of Natural Resources' permit issuance, which lacked prior informed consent from indigenous communities. Although the challenge was unsuccessful, it highlighted the need for alternative legal measures and systemic changes to protect the wild rice environment and indigenous rights. The Line 3 pipeline project revealed significant flaws in the implementation and design of RoN in the present legal framework, demonstrating broader patterns of sociocultural oppression and treaty rights violations.[1]

The Minnesota DNR's actions illustrated a failure to uphold legal pluralism, underscoring the necessity for a paradigm shift in environmental law advocating for judicial recognition of nature's rights and redefining health and sovereignty to align with indigenous perspectives.[2] As a signatory to international ecosystem initiatives, the United States has an ethical responsibility to uphold a pluralistic legal system. This case emphasizes the urgent need for legal reforms that genuinely protect the environment and respect indigenous sovereignty, advocating for transformative changes to ensure a sustainable future.[3]

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TP 18 and Poster 18

Synthesis and photophysical characterization of novel heterometallic Gold(I)-Copper(I) complexes

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The strategic selection of chromophores and their coordination with metal centers has a substantial impact on the emission characteristics of luminous materials. This study investigates the creative development and synthesis of a heterometallic complex that showcases a unique chromophore (2-ethynyltriphenylene), it is chosen due to its robust π-conjugation and inflexible planar structure, which greatly boost its capacity to absorb light and impact emission characteristics.[1] The chromophore is chemically bonded to a gold(I) core attached to a strong ligand, diphenylpyridine phosphine, which not only stabilizes the gold(I) center, but also enhances efficient electrical communication between the gold and copper centers due to its electron-donating properties and structural adaptability.[2] We examined the photophysical consequences of combining this gold(I) complex with five different copper(I) salts: $Cu(MeCN)_4PF_6$, $Cu(MeCN)_4OTF$, $Cu(MeCN)_4BF_4$, CuCl, and CuI, that enable the creation of diverse coordination environments and impact the photophysical characteristics of the complexes through metallophilic interactions.[3] The heterometallic assemblies underwent thorough characterization utilizing several techniques including NMR, FTIR, ESI-MS, X-ray crystallography, and various spectrophotometric techniques in solution, solid and matrices (PMMA, PS). This work offers an understanding of how changes in the copper(I) counterions affect the luminous characteristics of the complexes. It emphasizes the possibility of adjusting these characteristics by selecting the metal centers and their organic ligands with caution. This study adds to the overall comprehension of the connections between the structure and properties of heterometallic luminous complexes, which will facilitate specific improvements in optoelectronic applications.

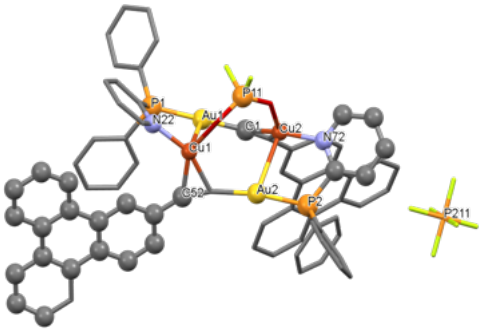

Figure 1. Crystal structure of ▪$CuPF_6$ complex with its heterometallic center

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TP 19 and Poster 19

Effects of leptin-derived peptides on β-amyloid folding patterns and aggregation inhibition

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Alzheimer's disease (AD) is a form of dementia that causes a gradual deterioration of brain function. One of the hallmarks of this disease is the deposition of amyloid plaques which result in neurofibrillary tangles, ending with cell death.[1,2] β-amyloid (Aβ) protein has long been known through its tendency to aggregate and form the amyloid plaques in extracellular regions of the brain.[3,4] The small fragments (peptides) of leptin have recently shown neuroprotective features, enhancing cognitive properties against AD. It has been assumed that one of the mechanisms that achieves this effect is through its inhibition of plaque formation in both intracellular and extracellular areas of neurons.[1,2]

The main aim of our study is to determine the mode of action of leptin-derived peptides in the aggregation process of β-amyloid. Thus, firstly we have studied the folding patterns of Aβ in its monomeric state. Although Aβ has been extensively calculated through various computational methods, it belongs to the class of intrinsically disordered proteins (IDPFs),[3] and the selection of the force field significantly affects its conformational behavior, for this reason, the reported results vary and are not conclusive of the folding patterns.[5] We have simulated the folding pattern of $A\beta_{42}$ through amber force fields, ff19SB and ff99DISP, under physiological conditions. Our results indicate that ff99DISP is the best suitable method to study the conformational landscape of Aβ. Additionally, we have studied the folding of this protein in presence of trifluoroacetic acid (TFA), in order to assess the effect of this counterion highly present in the experimental protocols, and leptin derived 9-residue peptide to study the change in the folding behavior. These results pave the way to a better understanding of different solvation or binding effects in the aggregation process of $A\beta_{42}$ and will be used to define synthetic modifications of the leptin-peptide moieties to improve the pharmacokinetics profile.

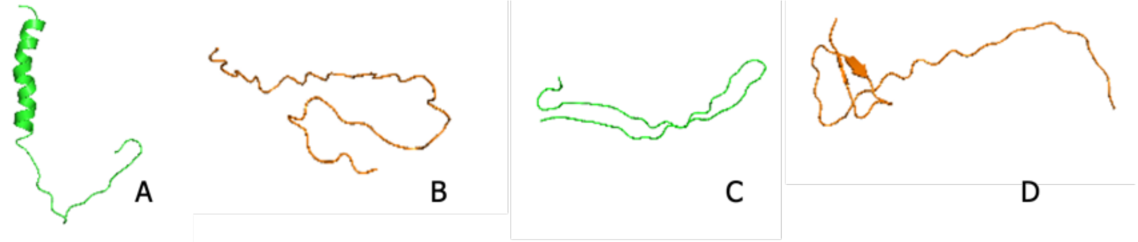

Figure 2. Snapshots of two equilibrated Aβ42 at the beginning of the simulations (A, B) and at the end of simulations (C, D).

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Safe and Sustainable by Design hybrid nanostructures, exploiting natural sources

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Naturally derived materials frequently exhibit intrinsic functional properties, including antimicrobial activity, and the ability to serve as stabilizers, dispersants, or carriers for other phases. *Halla parthenopeia*, a marine worm native to the Mediterranean Sea, produces two distinct types of mucus throughout its life: purple and colorless.[1,2] The purple mucus contains a red pigment known as 1,2-anthraquinone *Hallachrome*, which is toxic to bacteria, protozoans, rotifers, and crustaceans.[3] Colorless mucus facilitates locomotion and protects the worm from its own toxic purple mucus.[4]

This research focuses on combining products derived from H. parthenopeia with inorganic phases to develop hybrid nanostructures with a range of potential applications, from antibacterial to osteoconductive. For this purpose, Hallachrome has been combined with Hydroxyapatite to obtain Hydroxyapatite/Hallachrome (HAP/HAL) nanopowders, while purple and colorless mucus have been employed for the synthesis of gold (AuNPs) and silver (AgNPs) nanoparticles, respectively.

The process of HAP/HAL nanopowders synthesis involved the preparation of a hydroxyapatite suspension using the wet precipitation method at 37°C, followed by the addition of 1.3 mg, 0.7 mg, and 0.4 mg of Hallachrome dissolved in either DMSO or ethanol during the aging process. Silver and gold nanoparticles were produced by mixing $AgNO_3$ and $HAuCl_4$ with different volumes of mucus at room temperature for several days. The designed materials were characterized using various techniques, including XRD, FTIR, UV-Vis spectroscopy, SEM, and DLS. The antibacterial activity of the HAP/HAL nanopowders was tested against *S. aureus*.

HAP/HAL nanopowders exhibited antibacterial effects against *S. aureus* at Hallachrome concentrations of 1.2% and 0.6%. Both AuNPs and AgNPs were found to have a spherical shape, with average particle sizes ranging from 37-40 nm and 112-130 nm, respectively.

Overall, the results demonstrate the ability of biomaterials derived from H. parthenopeia to exhibit antibacterial effects (Hallachrome) and serve as reducing and stabilizing agents for the synthesis of gold and silver nanoparticles (purple and colorless mucus).

Acknowledgments: We would like to express our gratitude to Franco Corticelli for SEM images and Francesca Bonvicini for antibacterial testing. Also, we would like to thank the Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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TP 21 and Poster 21

Two-dimensional transition metal dichalcogenides for gas sensing applications

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Climate change is one of the most pressing global challenges of our time, with the emission of greenhouse gases (GHGs) being a significant contributor. To effectively combat climate change, accurate and reliable monitoring of these gases is crucial. Detecting GHGs like carbon dioxide, methane, nitrous oxide, and ozone constitutes the primary and principal phase in discovering solutions to effectively control and diminish the concentrations of these gases in the Earth's atmosphere.[1]

Traditional semiconducting metal oxides used in gas sensors have major limitations, such as high-power consumption, poor stability, limited selectivity, and sensitivity to humidity, hindering their efficiency in providing real-time data critical for climate change mitigation strategies.

Transition-metal dichalcogenides (TMDs), a class of 2D materials, have emerged as promising alternatives. These materials offer enhanced sensitivity, selectivity, stability, and response times due to their nanoscale thickness, large surface area, abundant active edge sites, and high sensitivity to gases even at lower temperatures, including room temperature.[2]

The focus of the thesis is the synthesis TMDs, (MoS_2, WS_2,) both in their pristine and functionalized forms, for advanced chemo resistive gas sensors. We investigate a novel and simple method of synthesizing these 2D layered materials with excellent scalability and reproducibility. A facile synthesis route was developed via a combination of liquid-phase exfoliation and lithium (Li) intercalation exfoliation to synthesized MoS_2 and WS_2. Additionally, the research explores a method to enhance the functionality of these transition metal dichalcogenides by functionalizing MoS_2 and WS_2 nanosheets with ZnO, SnO_2, and Pt nanoparticles via a simple solution mixing technique.

The synthesized and functionalized TMDs have been characterized using methods such as X-ray diffraction spectroscopy, field emission scanning electron microscopy (FESEM), and transmission electron microscopy (TEM) to validate their crystalline structure and morphology. Changes observed in the X-ray diffraction (XRD) pattern as a function of various solution processing durations confirm the production of few-layered TMDs. Also, we demonstrated a surface functionalization strategy for the TMD's with novel metal (Pt) and semiconducting metal oxides (ZnO, SnO_2).

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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TP 22 and Poster 22

Extended Triphenylene-based Metal-Organic Frameworks (MOFs) for Sustainable Catalysis

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Metal-organic frameworks are state-of-the-art crystalline, hybrid (organic-inorganic) materials, formed by the self-assembly of intricate units comprising transition metal centers interconnected by organic ligands, they represent a category of porous coordination polymers consisting of multidentate organic linkers bonded to a metal node.[1,2] These structures are promising for heterogeneous catalysis due to their high surface area and porosity. The research evaluates the catalytic properties of various two-dimensional (2D) MOFs based on extended triphenylenes functionalized with amine groups following their distinct advantages over 3D MOFs following potential for catalyst recovery and providing active sites due to their basic properties.[1,3]

The ligands are synthesized from Hexabromtriohenylne(**HBTP**) as precursor to form position 2,3,6,7,10,11-hexaaminitriphenylene (**m-HANT**), ortho position 2,3,6,7,10,11-hexaaminitriphenylene (**o-HANT**) synthesized through C-C cross-coupling reaction catalyzed by palladium(Suzuki-Miyaura method), and 2,3,6,7,10,11-hexakis(tert-butylamine) triphenylene (**HTAT)** ligand synthesized through C-N cross-coupling reactions catalyzed by palladium (Buchwald-Hartwig method). The ligands are characterized by the ^{1}H NMR.

The bottom-up approach was used to synthesize the MOFs and the following metal Cu (II), Ni (II), and Pd (II) salts are individually reacted with these extended triphenylenes. Characterization of the MOFs is performed using the following techniques infrared spectroscopy (IR) for functional group analysis, powder X-ray diffraction (PXRD) for crystallinity assessment, and scanning electron microscopy (SEM) for morphology determination. Finally, the catalytic performance of the MOFs is evaluated in the Suzuki-Miyaura reaction using Natural Deep Eutectic Solvents (NADES) as the reaction medium.

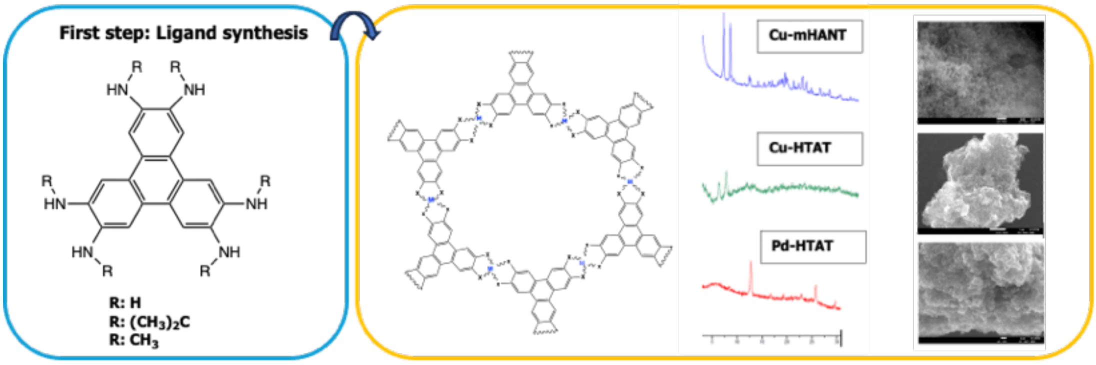

Figure 3: MOFs synthesis and Characterization(PXRD,SEM) scheme

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR) grant agreement nr 619824-EMJMD

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Towards the generation of full AMPK model combining experimental and computational techniques

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Mammalian AMP-activated protein kinase (AMPK) plays a critical role in cellular energy homeostasis and has emerged as a key therapeutic target for several diseases, mainly related to metabolic and cardiovascular disfunctions. AMPK possess a heterotrimeric structure, expressed in distinct isoforms of α, β, and γ subunits.[1] The different combination allows up to 12 distinct AMPK complexes with tissue-specific distributions and metabolic functions. However, the absence of a fully crystallized system has been an impediment to understand the activation mechanism of AMPK, which has been described as: i) allosteric, ii) indirect, and iii) direct, where several domains of the different subunits are directly related. Therefore, to effectively design a selective drug for a specific AMPK complex, it is essential to understand its conformational plasticity and biological structure.

The present study is focused on the α2β2γ1 AMPK complex, which is the most abundant one in the skeletal muscle, and thus an important therapeutic target for Type 2 Diabetes Mellitus (T2DM). Therefore, the main objective of this project is to obtain a reliable 3D full model for α2β2γ1 AMPK.

By combining experimental data analysis[2] and *in silico* techniques, such as Multiple Sequence Alignment and Homology Modeling, we were able to obtain two reliable models for the targeted complex. The present work represents a significant advancement in AMPK research, bridging the gap between experimental studies on the full system and computational analyses of isolated structural domains.[3] The resulting 3D models of the α2β2γ1 AMPK complex provides fruitful insights into the allosteric activation mechanism of AMPK, potentially facilitating the design of specific modulators for this complex.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Total polyphenols in commercial foods: quantification and computational analysis as an integral part of the mediterranean diet framework

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Emerging evidence highlights the intricate relationship between total polyphenol content (TPC) in various food and beverage samples and their significant contributions to health-promoting outcomes, serving as major sources of phenolic compounds. This study aims to quantitatively analyze the TPC in commercially available food and beverage samples. Additionally, it employs the Phenol-Explorer database to obtain a list of polyphenol metabolites for conducting a computational study on their interactions with biological targets. Our focus encompasses high-polyphenol items such as herb infusions, teas, vegetable milks, soya sauces, vegetable soups, and coffees. By integrating quantitative and computational analysis, we effectively quantify polyphenol levels and advance a predictive framework for their molecular interactions. This approach broadens the scope of polyphenol research in nutritional science and underscores the health benefits associated with the Mediterranean diet.

Our study employs the Folin-Ciocalteu method with gallic acid equivalents for precise quantification of total polyphenols in food and beverage samples, reflecting actual consumption patterns. Sample preparation includes stepping, cooling, and diluting, mimicking typical culinary practices. UV-VIS spectrophotometry at 765 nm, supported by gallic acid calibration curves, ensures accuracy. Complementarily, our computational analysis rigorously models the interactions between polyphenols and specific biological targets (Tight juchtion protin (Occludin and Zonulin) Leptin and Titin), providing deeper insights into their potential therapeutic effects and health benefits.

Statistical analysis identified significant variations in total polyphenol content (TPC) across six food groups ($p<0.05$). Specifically, coffees and vegetable milks exhibited the highest TPC (mg/per surving of food) compared with herb infusions, teas (red, black, green), vegetable soups, and soya sauces. After categorizing the samples, they were further analyzed in quintiles of ten samples each, which revealed distinct variations in TPC ((mg/per surving of food) across the groups. Computational studies revealed that polyphenols such as theaflavin and (-)-epigallocatechin 7-O-glucuronide exhibited notable interactions with protein targets, including Tight Junction Protein (TJP) and Titin, suggesting potential health benefits through these specific bindings.

This research underscores the integration of analytical and computational methodologies as a robust approach to investigate the health-promoting properties of polyphenols within the context of the Mediterranean diet. By quantifying total polyphenol and their interactions with biological targets, the study provides a deeper understanding of how dietary polyphenols contribute to health benefits.

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Formation of pullulan-pectin hybrid gels for the obtaining of pullulan beads by dripping method. Rheological study and evaluation as active ingredient release systems

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Pullulan is a polysaccharide of plant origin. Although it has attracted attention as a biofilm former with the ability to increase the shelf life of foods, its ability to form hydrogels has not been investigated in depth. It presents slow cross-linking kinetics with sodium trimehaphosphate (STMP), in such a way that it allows obtaining hydrogels in bulk form but the formation of beads by the dripping method is not possible, as dissolution of droplets occurs before gelation. Obtaining hybrid gels using another polysaccharide, in this case pectin, a polymer that does not cross-link with the same cross-linking agent as pullulan, has been evaluated. Using rheological measurements, the minimum concentration of cross-linking agent needed to form hybrid gels has been studied. It has been observed that when pectin has been added to the solution of pullulan, the minimum STMP necessary for gelation was 90% lower than without the presence of pectin. The gelation time of the hybrid gels has also been evaluated, being this time practically instantaneous, thus allowing the obtaining of beads by dripping of the polysaccharide solution in an aqueous solution of the gelling agent. The properties of hybrid gels prepared in bulk have been studied by rheology, by microscopy (SEM) and by analysing their swelling degree and water retention capacity. Finally, beads have been formed by the dripping method, loaded with gallic acid as a model to evaluate their suitability as delivery systems for active ingredients. The release profiles show that they were systems comparable to beads formed by other biopolymers and therefore capable of adequately releasing active ingredients.

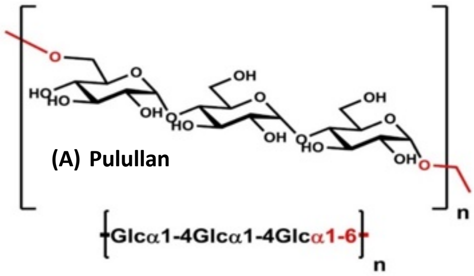

Figure 1 Chemical Structure of Pullulan[1]

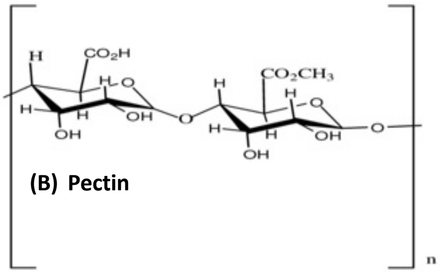

Figure 2 Chemical Structure of Pectin[2]

Acknowledgments: I would also like to express my sincere appreciation to the Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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