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Book of Abstracts

Plenary Talks

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Quantum Dots Produced by Pulsed Laser Ablation in Liquids: A Sustainable Route Toward Advanced Functional Nanomaterials

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The development of advanced functional nanomaterials with tailored optical, electronic, and chemical properties is central to emerging technologies in energy conversion, sensing, photonics, and biomedicine. Among these materials, quantum dots have attracted considerable attention because of their size-dependent electronic structure, tunable emission characteristics, and strong light–matter interactions. However, conventional chemical synthesis methods often require complex reaction schemes, toxic precursors, and surface ligands that can limit material performance and environmental sustainability.

This plenary lecture will present pulsed laser ablation in liquids (PLAL) as a versatile and environmentally friendly platform for the synthesis of high-purity quantum dots [1] and nanostructured materials. By exploiting the extreme nonequilibrium conditions generated during laser–matter interactions, PLAL enables the direct production of ligand-free colloidal nanomaterials with clean and highly reactive surfaces. Recent advances in the synthesis of semiconductor quantum dots and related nanostructures will be discussed, highlighting the influence of laser parameters, liquid environment, and post-synthesis aging on particle size, morphology, crystal structure, and optical properties.

Particular emphasis will be placed on the relationship between nanoscale structure and functionality, including quantum confinement effects, photoluminescence behavior, charge transport, and interfacial phenomena. Examples involving chalcogenide-based nanomaterials [2] and emerging quantum materials will illustrate how laser-based synthesis can produce colloids with remarkable long-term stability while preserving surface activity. The opportunities offered by these materials for flexible optoelectronics, photocatalysis, and next-generation photonic devices will also be explored.

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This work was supported by the National Science Foundation (NSF) under Grant No. 2228891 and under Grant No. 2533178.

THE MULTIFACETED CHEMISTRY OF AROMATIC PHOSPHORUS HETEROCYCLES

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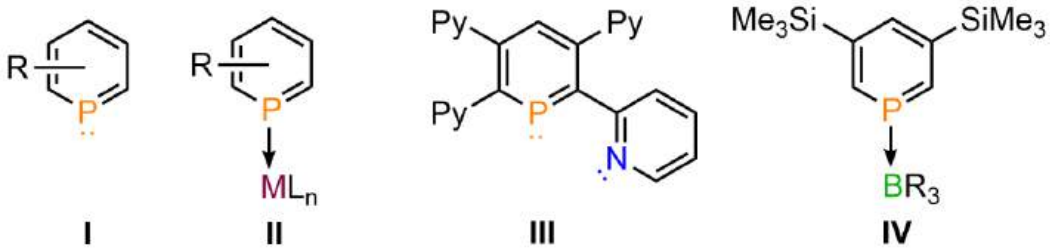
Phosphinines (**I**), the higher homologues of pyridines, are known since the pioneering work of Märkl [1]. Due to their pronounced π-accepting properties, phosphinines have been predominantly used for the synthesis of coordination compounds (**II**), in which the metal center displays a low oxidation state [2]. Even reduced metal complexes have been reported. Moreover, several substituted phosphinines have been used as phosphorus ligands in homogeneous catalytic reactions [2].
We have recently started to explore such low-coordinate, aromatic phosphorus heterocycles in metal-free small molecule activation, making use of P,N-cooperativity (**III**) [3]. Furthermore, the Lewis pair **IV** shows a remarkable behavior towards certain substrates due to a dynamic reactivity [4].



I **II** **III** **IV**

We report here particularly on the reversible reaction of **III** with H_2O, the reaction of **IV** with iso(thio)cyanates and the application of **IV** as main-group catalyst for the selective scrambling of phenylstannanes [4,5].

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Synthetic Cluster Models of Inorganic and Organometallic Active Sites in Proteins

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Complex inorganic active sites perform challenging catalytic transformations in biological systems, such as water oxidation by photosystem II and nitrogen reduction in nitrogenase. The effect of cluster structure on the physical and chemical properties of these active sites is not well understood. We have developed methodologies for the rational synthesis of homo- and hetero-metallic cluster models of protein active sites, which allow for systematic structure-property studies. Distal redox and ligand changes have been demonstrated to have a substantial effect on the reactivity and binding of ligands relevant to small molecule conversions. Carbon-based bridging ligands have been incorporated to probe potential effects of the interstitial carbide in nitrogenase, and were found to have a profound effect on electronic structure. Spectroscopic studies of models with structures or redox states relevant to the protein active site provide benchmarking for the biological systems. Implications for function and spectroscopy will be discussed.

FIBROUS POLYMER HYDROGELS: A NEW PERSPECTIVE ON MECHANICAL AND TRANSPORT PROPERTIES

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Fibrillar networks are ubiquitous in nature, however their biologically relevant properties are rarely recapitulated in man-made polymer hydrogels. This talk will highlight the unique behavior of fibrous polymer hydrogels under confinement, along with the role of structural anisotropy in the mechanical and transport properties of fibrous hydrogels.

References

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A Menagerie of Chemical Beasts and Their Strange Cages

Jonathan R. Nitschke

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Simple organic subcomponents can come together around metal-ion templates to produce intricate hollow capsules.[1] This talk will describe the design and uses of some of these three-dimensional architectures, a few of which are shown in Figure 1 below, along with the use of the same construction principles to produce interlocked structures – catenanes[2] and knots[3] – and double-helical metallopolymers with potentially useful optoelectronic properties.[4]

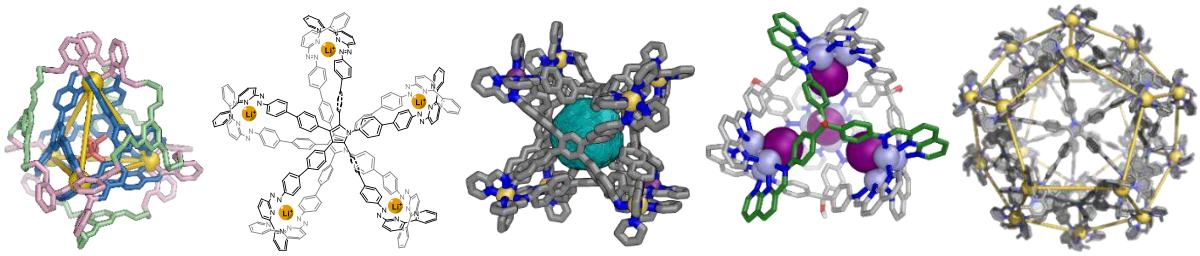

Figure 1. From left to right: a knotted capsule that exchanges guests 17000 times more slowly than its non-knotted counterpart;[5] a photoactive $Li_5L_2^{5+}$ complex that can extract Li^+ selectively from mixtures of the other alkali metals, and release it photochemically;[6] $Zn^{II}_8L_6$ with walls that dynamically expand to adapt to different guests; [7] a tetrahedral cage with Ag^{I}_3I vertices;[8] a dodecahedral capsule, congeners of which enclose enough interior volume to house a small protein.[9]

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From Optoelectronics to Solid Lubricants: The Multifunctional Potential of Sputtered δ-Bi_2O_3

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Bismuth oxide (Bi_2O_3) and related bismuth-based materials are highly versatile systems whose complex lattice structures drive their utility across diverse technological fields. Their tunable band gaps and exceptional oxygen-ion conductivity have made them a focal point for optoelectronics, gas sensing, and, notably, advanced photocatalysis. Yet, while these electronic and catalytic applications are well established, the cubic-defective fluorite-like δ-Bi_2O_3 phase offers compelling, underexplored potential in surface engineering. Interestingly, the same fundamental characteristics that govern its functional behavior—specifically, a highly defective crystal lattice—also dictate its unique mechanical and tribological responses.

This talk explores the targeted synthesis and functional characterization of δ-Bi_2O_3 thin films, bridging the gap between their optical and catalytic properties and their mechanical performance. Utilizing magnetron sputtering, we successfully stabilized the elusive δ-phase on AISI D2 steel substrates. We will detail the deposition parameters crucial for isolating this specific structural phase and discuss how the synthesis strategies influence the final film architecture.

Following successful synthesis, we evaluated the tribological response of the δ-phase coatings using pin-on-disk tests from room temperature up to 300 °C. The films exhibited exceptional solid-lubricant behavior, achieving low wear and coefficients of friction (COFs) between 0.05 and 0.15. To explain these uniquely low values, we propose a mechanistic model based on the coating's architecture: the intrinsic 25% anionic vacancies within the defective fluorite lattice—the same vacancies that enable high ionic mobility and drive surface reactivity—order to form low shear-strength planes, behaving remarkably similarly to Magnéli phases.

Finally, we will address the transitional hurdles for integrating these thin films into broader industrial applications. By examining the current challenges of substrate adhesion and thermal phase stability, we will highlight the next frontiers in synthesizing Bi_2O_3 composite coatings and engineering the next generation of lubricious solids.

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FROM CATALYST DEVELOPMENT TO CO_2 CAPTURE MATERIALS. HOW GUILTY LIGANDS ENABLE INNOVATION

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1,3-N,O-Chelated early transition metal complexes show unique reactivity for the direct catalytic addition of amines to alkenes by hydroaminoalkylation. State-of-the-art catalysts from the Schafer group feature N,O-chelating ureate ligands (Figure 1), with tuneable steric and electronic features, and flexible bonding modes, to enable efficient C-H bond activation and Csp^3-Csp^3 bond formation. Notably, there are many catalysts with N,O-chelating ligands, including well known modular phenoxyimine monoanionic ligated early transition metal complexes, that we know are not useful for hydroaminoalkylation catalysis. What is so special about this 1,3-N,O-chelating motif and how can these features be harnessed to optimize catalyst performance? This presentation will highlight structural, spectroscopic and computational insights that clarify the electronic and dynamic features of these ligands that are crucial for enabling challenging C-H bond activation reactions for C-C bond forming reactions with 100% atom economy, such as hydroaminoalkylation. Furthermore, we will use these mechanistic insights to rationalize hydroaminoalkylation as a regio- and diastereoselective green catalytic technology for generating complex small molecules, N-heterocycles, and amine-containing functional materials. Finally, we will show how simple commodity polyolefins can undergo catalytic amination to generate a new class of recyclable polymeric materials for CO_2 capture and release.

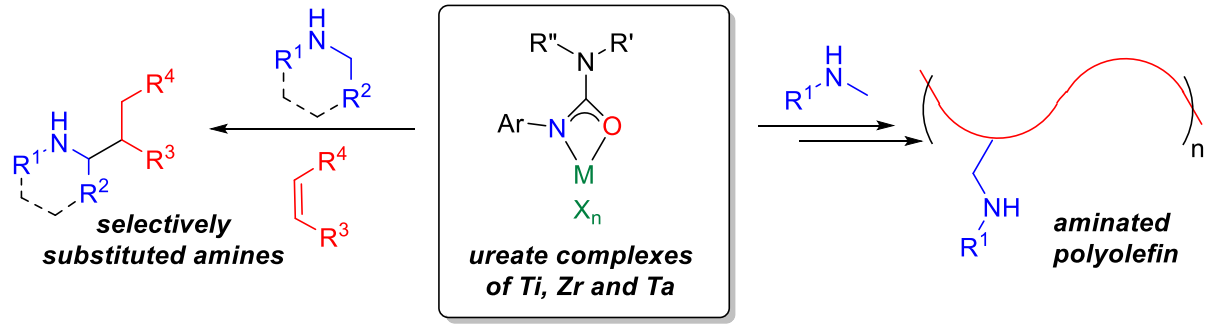

Figure 1. Modular ureate early-transition metal hydroaminoalkylation catalysts for the synthesis of small molecules and materials.

Session 1. Functional Polymers and Organic Materials

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INFLUENCE OF THE ORDER OF HONEY AND CITRIC ACID INCORPORATION ON THE STRUCTURE AND SWELLING PROPERTIES OF CHITOSAN MEMBRANES

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Abstract

Biopolymer membrane technology has emerged as a sustainable alternative to the use of petroleum-derived synthetic polymers in various environmental and industrial applications. Among the biopolymers of greatest interest is chitosan, owing to its biocompatibility and biodegradability. However, its mechanical properties limit its functionality and can therefore be improved through the incorporation of crosslinking agents and plasticizers. Citric acid represents a lower-environmental-impact alternative to toxic agents such as glutaraldehyde, while the incorporation of naturally derived plasticizers, such as honey, allows the molecular mobility and hydrophilicity of the polymer matrix to be modified [1]. The present study aimed to evaluate the effect of the concentration and incorporation order of honey and citric acid on the swelling and permeability properties of chitosan membranes, with the purpose of establishing formulation conditions that promote the formation of a stable polymer network with controlled functionality. The membranes were prepared using the casting technique, employing different formulations with varying concentrations of honey and citric acid, as well as different sequences of additive incorporation. The membranes exhibited differences in color, thickness, and surface texture. The average thickness increased upon incorporation of the plasticizer. FTIR analysis revealed changes in the absorption bands of the functional groups within the matrix, associated with the formation of interactions between chitosan and citric acid. The formulation obtained through the simultaneous incorporation of honey and citric acid exhibited a maximum swelling factor of Sf = 3.71. The prior addition of honey to the crosslinking agent may promote partial shielding of chitosan functional sites, thereby limiting its interaction with citric acid. Likewise, high concentrations of the components may compromise matrix stability. These results demonstrate that controlling the composition and incorporation sequence of the modifiers constitutes an effective strategy for tailoring the structure and functional properties of the membranes, making these materials promising candidates for separation, species transport, and controlled-release applications.

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Physicochemical properties of *Guadua aculeata* carbon as a photothermal material for water purification

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Biomass represents an abundant and sustainable carbon-rich precursor that, when subjected to thermochemical treatments in oxygen-deficient atmospheres, transforms into biochar possessing high thermal stability, hierarchical porosity, and remarkable capillarity [1]. These features facilitate efficient solar energy conversion, positioning biochar as a promising, low-cost candidate for photothermal water purification and desalination devices [2]. In this study, the physicochemical properties of bamboo stalks (*Guadua aculeata*) harvested in Hueytamalco, Puebla, Mexico, were systematically evaluated along with their structural and surface evolution following carbonization at 400 °C and 500 °C. Elemental analysis of raw biomass indicated a lignocellulosic matrix dominated by cellulose (46%), hemicellulose (21%), and lignin (20%), with 43% elemental carbon and 10% ash. Fourier-transform infrared spectroscopy (FTIR) and thermogravimetric analysis (TGA) confirmed the progressive thermal degradation of oxygenated functional groups (C=O, C–O) and cellulose with increasing temperature. X-ray diffraction (XRD) demonstrated a transition from a semi-natural cellulosic structure to ordered amorphous carbonaceous phases at 500 °C, while SEM imaging verified the preservation of a native porous hierarchy (micropores and nanopores) crucial for fluid transport. ICP-OES elemental profiling revealed notable concentrations of silicon (Si) and potassium (K), with Si content decreasing at higher temperatures due to inorganic matrix rearrangement. Contact angle measurements demonstrated structural anisotropy in wettability: hydrophobic behavior along longitudinal cuts (greater than 90 ° in both carbons) versus hydrophilic behavior across cross-sectional cuts (less than 90 °). This unique amphiphilic balance, coupled with thermal stability and porous architecture, positions *Guadua aculeata* charcoal as an effective material for driving capillary transport and interfacial solar evaporation.

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Acknowledgements

Thank you very much to INIFAP for supporting the collection of bamboo materials.

Abstract preparation

A FLEXIBLE CAPACITIVE PRESSURE SENSOR BASED ON FOOD-GRADE XANTHAN GUM: MECHANICAL ENHANCEMENT MATERIAL FOR DIELECTRIC GEL

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The development of pressure sensors for biomedical and E-skin applications has expanded in recent years. The operation of these devices is based on various electrical phenomena, such as piezoelectric, resistance and electrical capacitance. Mechanical, electrical and chemical properties of organic materials have been employed to develop capacitive pressure sensors, leveraging the easy processability of these materials to develop simple devices. This work presents a study of the flexible pressure sensor consisting of an electric double-layer capacitor, which comprises a semi-aqueous dielectric layer supported by PVA, silver nanowires and food-grade xanthan gum. Due to its water retention and mechanical properties which are enhanced by the presence of PVA, xanthan gum enables the production of a gel that can be compressed at low pressures. These devices achieving a capacitance of 300 μF and capable of measure pressure differences ranging from 196 to 3000 Pa, achieved. A sensor device based on capacitance responses from an organic material was developed using low-cost materials and simple fabrication methods, potentially enabling applications such as electronic skin, among others.

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Optimizing Doxorubicin Encapsulation in Pluronic® P104 Micelles through Control of Temperature and Drop Rate

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Doxorubicin (DOX) is a widely used chemotherapeutic agent, but its clinical use is limited by its lack of selectivity and dose-related toxicity. Improving its encapsulation in polymeric micelles may provide a strategy to optimize its incorporation into these delivery systems. Pluronic® amphiphilic PEO-PPO-PEO triblock copolymers are promising drug delivery systems due to their biocompatibility and self-assembly into micelles with a hydrophobic PPO core and hydrophilic PEO shell, enabling the encapsulation of poorly soluble drugs [1]. In this study, we investigated the formation, stability and DOX loading capacity of Pluronic® P104 micelles. Micellization and morphological transitions were first characterized by dynamic light scattering using temperature ramps (10-64 °C). To identify optimal conditions for DOX encapsulation within the micellar core, hydrophobic doxorubicin free base (DOXO-B) was synthesized from commercially available DOXO-HCl using an optimized triethylamine/dichloromethane protocol, yielding 65.85 ± 3.91%. Using the synthesized DOXO-B, we then evaluated the effect of formulation conditions on encapsulation efficiency (EE) and the formation of a homogeneous micellar population, identifying temperature and water addition rate as key parameters. Preparation at 40 °C, above the CMT of P104, promoted the initial hydrophobic interactions between DOXO-B and the dehydrated PPO blocks, increasing EE from 19.4% to 47.6% at an initial DOXO-B concentration of 50 µg/mL (Fig. 1), as determined by UV–Vis spectroscopy. It was also determined that a slow and controlled addition of DOXO-B and water further promoted drug incorporation while limiting aggregate formation. Overall, these findings demonstrate that preparation conditions, specifically encapsulation temperature and water addition rate, significantly impact drug loading capacity.

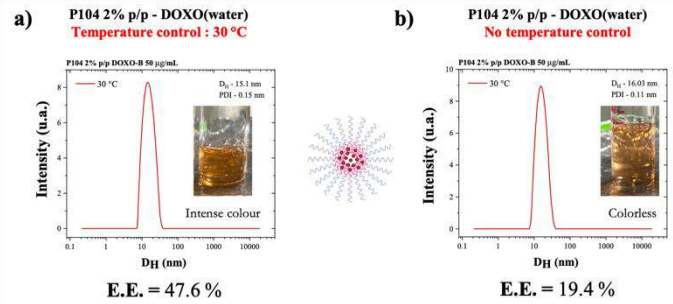

Figure 1. *Effect of temperature on micelle formation and DOXO-B incorporation.*

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Optical and Morphological characterization of thin films of an organic semiconductor material from Schiff bases

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Condensation reactions are efficient mechanisms for the synthesis of π-conjugated systems. In particular, these reactions are fundamental in the synthesis of Schiff bases to obtain π-conjugated systems by efficiently connecting diverse functional groups through imine bonds (C=N), thereby achieving electron delocalization throughout the entire structure.

On the other hand, azo compounds possess N=N bonds that can extend π-conjugated systems while providing the ability to undergo photoisomerization/isomerization, triggering a change in their spatial geometry. These properties are particularly attractive for the design of novel materials with potential semiconductor applications.

In this work, we report the synthesis of a novel molecule, 4-((E)-(4-(((E)-3,5-dibromobenzylidene)amino)phenyl)diazenyl)-N,N-dimethylaniline, which was evaluated for its semiconductor properties. The compound was characterized using spectroscopic techniques such as FT-IR and NMR to confirm its chemical structure and purity. Additionally, its optical properties were investigated by UV-Vis absorbance and fluorescence emission spectroscopy in solution, allowing the evaluation of both the Stokes shift and the optical bandgap energy. Finally, thin films were prepared using two distinct techniques: spin coating and Physical Vapor Deposition (PVD). The morphology, roughness, and homogeneity of these films were subsequently characterized by Atomic Force Microscopy (AFM).

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Effect of power and irradiation rate on laser induced graphene structure from commercial polyimide

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Nowadays with the growth of portable devices market, flexible devices have gained increased attention from researchers and technologist. Thus, the use of polymers for such flexibles devices due to their mechanical, optical and versatile properties is very attractive.

On the other hand, graphene has shown great potential for flexible devices because of its exceptional mechanical and electrical properties. Nevertheless, the chemical synthesis of graphene usually requires multiple steps and highly corrosive and oxidative reagent such as H_2SO_4 and $KMnO_4$. As alternative, Laser Induce Graphene (LIG) has emerged, in which a polymer substrate is scribed with a laser to form graphene in a single step, this process is rapid, cheap, more environmentally friendly, scalable and LIG is obtained on a flexible polymer substrate.

Therefore, in this work, the effect of the laser power and irradiation rate in the structure of the obtained graphene from commercial polyimide was studied. SEM technique was used to evaluate the structure of graphene while energy dispersive spectroscopy (EDS) helps confirmed the mechanism formation reported by other authors. Furthermore, Raman spectroscopy was used to evaluate the quality of graphene and the mechanism process. Additionally, it was found that specific combination of laser power and irradation rate produced three main types of morphology: graphene sponge, hierarchical porous carbonaceous structures, and carbon fibres.

These results show a great potential for application in flexible electronics, such supercapacitors, flexible sensors, hydrogen generation, membrane separation and other technologies.

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STUDY OF THE FORMATION, CHARACTERIZATION AND STABILITY IN THE PRESENCE OF BIOLOGICAL MOLECULES, OF PLL/DNA COMPLEXES FOR GENE THERAPY

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In recent decades, natural and synthetic cationic polymers have been extensively investigated as non-viral carriers for nucleic acid-based therapeutics. These polymers act through electrostatic association with DNA or RNA molecules, leading to the formation of supramolecular assemblies known as polyelectrolyte complexes. Among them, lysine-based polymers such as poly-L-lysine (PLL) have attracted considerable interest due to their biocompatibility, ease of synthesis, and chemical modifiability [1]. However, a comprehensive understanding of the physicochemical mechanisms governing complex assembly and disassembly, stability in biological media, and intracellular nucleic acid release remains lacking [2]. In this study, poly-L-lysine (PLL) with degrees of polymerization ranging from 20 to 2,400 was evaluated as nonviral gene delivery vector using the eGFP-C3 plasmid DNA as a model nucleic acid. Complexes were formed at four different charge ratios (R=$[N^+]/[P^-]$): 3, 5, 10, and 15. The resulting formulations exhibited hydrodynamic diameters below 100 nm, positive surface charges, and excellent colloidal stability for up to 7 days. Additionally, the amount of heparin required to release DNA increased with charge ratio, reflecting the greater stability of polyplexes formed at higher R values. Transfection assays demonstrated efficiencies up to 35% after 72 hours (**Fig. 1a** and **1b**) while maintaining cell viability above 90%. These results highlight the potential of PLL as a promising nonviral vector for gene delivery.

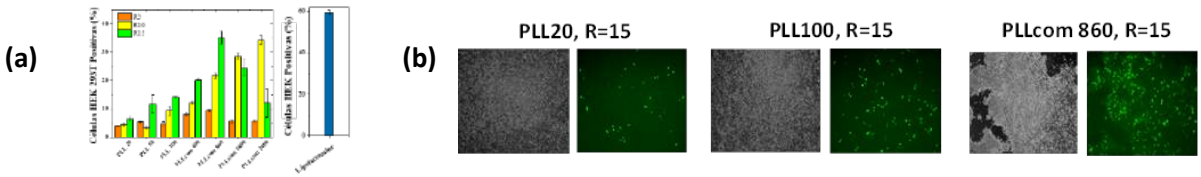

Fig. 1. Evaluation of GFP expression in HEK293T cells 48 h after transfection with PLL/DNA polyplexes by **(a)** flow cytometry and **(b)** fluorescence microscopy.

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Physicochemical Insights into Chitosan-Insulin Complex Formation and Stability

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Oral administration of insulin remains a major challenge in diabetes therapy due to the poor stability and limited absorption of the protein in the gastrointestinal tract [1]. Chitosan-based polyelectrolyte complexes have emerged as promising systems for improving insulin protection and delivery. In this work, we investigated the formation, physicochemical properties and temporal colloidal stability of chitosan-insulin complexes prepared using chitosans with different molecular weights (MW). Three chitosan samples were studied, with MW of 35, 87 and 417 kg/mol. The electrostatic interactions governing complex formation were first investigated using ζ-potential titrations. Chitosan-insulin complexes were prepared at different chitosan-to-insulin charge ratios (R), *i.e.* from 0.5 to 15. Their size, polydispersity, surface charge and morphology were characterized using Dynamic Light Scattering (DLS), ζ-potential measurements, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). We found that at R ≤ 2, complexes formed monodisperse nanoparticles with sizes below 110 nm, demonstrating the formation of well-defined nanoscale complexes. The ζ-potential increased progressively with R, from approximately +10 mV at R = 2 to +23 mV at R = 15. SEM and TEM imaging allowed a direct visualization of the complexes, revealing predominantly compact particles in the nanometer size range. Among the complexes studied, the medium-molecular-weight chitosan-insulin complex prepared at R = 2 exhibited the highest stability over time, maintaining its colloidal properties for up to 3 days, whereas low-molecular-weight chitosan-insulin complexes were less stable. Overall, these results highlight the role of charge ratio and chitosan MW in determining the stability of chitosan-insulin complexes and provide useful guidance for their optimization as protein delivery systems.

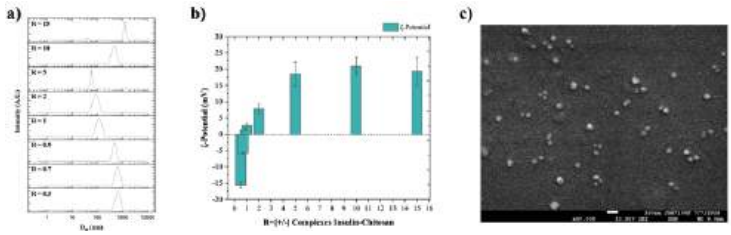

Figure 1. *Characterization of insulin-high-MW chitosan complexes. (a) Hydrodynamic diameter distributions at different charge ratios (R). (b) ζ-potential as a function of R. (c) SEM image of complexes at R = 2 (scale bar = 100 nm).*

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IMPACT OF THE ARCHITECTURE ON GELATIN-CHITOSAN HYDROGELS SYNTHESIZED BY GAMMA RADIATION FOR BIOMEDICAL APPLICATIONS

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Gelatin (GE) and chitosan (CS) hydrogels are widely used biopolymers in biomedical applications due to their biocompatibility, biodegradability, and functional properties. However, they are limited by their mechanical stability. In this study, two systems based on GE/CS architectures were synthesized by gamma radiation: a comb-like grafted hydrogels (*net*-GE)-*g*-CS and a composite hydrogel reinforced with chitosan nanogels (*net*-GE/*net*-nCS). Optimal synthesis conditions were established at 3% w/v of GE, 1.5 % w/v of CS or *net*-nCS, and a 15 kGy dose. FTIR and thermal analyses confirmed CS incorporation, while structural analysis revealed differences associated with covalent grafting in comb-like hydrogel and non–covalent interactions in composite hydrogel. Swelling studies showed that comb-like hydrogels reached equilibrium faster and exhibited reduced water uptake when high CS concentration was used, whereas composites exhibited moderate swelling reduction and both systems showed pH-responsive behavior with a critical pH of 2.7. Mechanical characterization showed a significant increase in stiffness for (*net*-GE)-*g*-CS compared to composite and *net*-GE. Drug loading and release studies using diclofenac showed superior retention and release efficiency in composite hydrogels, attributed to the presence of swollen chitosan nanodomains. The results demonstrate that hydrogel architecture critically influences physicochemical and drug delivery properties.

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CUSTOM-SYNTHESIZED PS-b-PMMA COPOLYMERS VIA ULTRASOUND

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The synthesis of block copolymers (BCPs) from polymers via ultrasound (US) catalysis offers an alternative to traditional thermomechanical recycling, given the significant environmental and economic importance of polymer reuse. BCPs are highly versatile, serving roles ranging from compatibilizers for polymer blends to nanomaterials for a multitude of cutting-edge technological applications [1,2]; this versatility stems from their ability to self-assembly into various geometries—such as lamellae, cylinders, spheres, etc.—depending on their composition when deposited as thin films [3].

PS-b-PMMA copolymers were synthesized by varying reaction conditions (frequency, solvent, polymer ratio, and molecular weight). Reaction yields were low (<10%) and decreased as the amount of PS in the reaction increased. ^{1}H and DOSY-NMR analyses confirmed the production of BCPs with varying PS/PMMA ratios and the synthesis of AB-type BCPs, respectively; FTIR qualitatively confirmed the proportions, while HPLC-SEC indicated the formation of both monodisperse and polydisperse BCPs with low molecular weights (<50 kDa). While US-assisted chemical recycling of these polymers is a promising route to obtaining higher value-added materials [4,5], a better understanding of the reaction mechanism is still required to improve yields and ensure economic feasibility.

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Incorporation of mechanically recycled PET into food packaging applications: Impact of Contaminants

Christelle Combeaud, Jean-Luc Bouvard, Joulia Housseini

Mechanical recycling of polyethylene terephthalate (PET) has become a strategic priority for the food packaging sector, driven by increasingly stringent European directives requiring higher collection rates and greater incorporation of recycled PET (rPET) into food-contact packaging. Despite these advances, the presence of residual contaminants, notably polyole ns such as polypropylene (PP) and printing ink residues, remains a major obstacle to the production of high-quality recycled materials. These impurities can substantially modify the physico-chemical and mechanical behaviour of rPET, thereby compromising its processability and the performance of the nal food packaging products.

This research, carried out in collaboration with CEMEF–Mines Paris and SIDEL, aims to elucidate the in uence of polyole n and ink contaminants on the structure–property–processing relationships of recycled PET. Particular emphasis is placed on understanding the individual and combined effects of PP and ink residues on the microstructural evolution, crystallization kinetics and mechanical behaviour of rPET under processing conditions representative of industrial manufacturing, with a specific focus on injection stretch blow moulding (ISBM).

To this end, a series of rPET formulations containing controlled concentrations of contaminants are produced and systematically characterized using a multi-technique experimental methodology. Structural and molecular modifications are investigated through X-ray diffraction (XRD) and differential scanning calorimetry (DSC) to quantify changes in crystalline morphology and molecular organization. The thermo-mechanical response is analysed thanks to dynamic mechanical analysis (DMA) so as to identify the forming range. The stretchability of the material is assessed through uni-axial tensile tests, in the rubbery-like state, reproducing the thermo-mechanical conditions encountered during the stretch blow moulding process.

The outcomes of this study are expected to provide a comprehensive understanding of the mechanisms by which polyolefin and ink contaminants affect the processing and performance of recycled PET throughout ISBM process. Beyond advancing the fundamental knowledge of contaminated polymer systems, this work seeks to identify processing strategies and material optimization approaches that improve the industrial recyclability of PET, facilitating the integration of higher rPET contents into food packaging applications.

This study investigates the effects of polypropylene and ink contaminants on the structure, properties, and processability of recycled PET, with the aim of optimizing its use in food packaging and improving industrial performance.

Different rPET grades containing controlled PP and ink contamination levels are characterized by XRD, DSC, DMA and tensile testing to correlate structural, thermal, and mechanical changes with processability under industrial ISBM process. The presence of contaminants tends to retard rPET crystallization under both static and dynamic conditions, thereby affecting material processability and deformation during injection stretch blow moulding.

DEVELOPMENT AND EVALUATION OF BIOPOLYMERIC COATINGS OF CHITOSAN FUNCTIONALIZED WITH CHIA OIL FOR BLACKBERRY PRESERVATION

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Abstract

In Mexico, the annual production is estimated at approximately, of which around 70% corresponds to waste, mainly shrimp exoskeletons [1]. Due to their chitin content, this waste represents a potential source for obtaining chitosan and its utilization in the development of materials with applications in food. In this study, coatings were developed incorporating chia oil for application on berries, specifically blackberries [2].

Chia seeds (Salvia hispanica) were acquired in San Mateo Atenco, Puebla, and the oil was obtained through an extrusion process, achieving a yield of 25% (w/w). Subsequently, the effect of the application and preservation conditions of the coating on the antioxidant activity of blackberries was evaluated using a 2^3 factorial design. The factors studied were storage temperature (5°C and 25°C), immersion time (5 and 10 seconds), and chia oil concentration in the coating (0% and 3%). Antioxidant activity was determined using the DPPH assay after one and two weeks of storage.

During the first week, antioxidant activity values ranged between 46.0-60.6% inhibition. All factors individually had a significant effect on antioxidant activity ($P<0.05$), while interactions between factors did not show statistically significant effects ($P>0.05$). The factor that most influenced antioxidant activity was the storage temperature.

After two weeks of storage, antioxidant activity values ranged between 30.9-88.2% inhibition. During this period, all three factors showed significant effects on antioxidant activity, as did the interactions between temperature-chia and immersion time-chia ($P<0.05$). The variable that most affected antioxidant activity during the second week was the chia concentration. It was observed that at a storage temperature of 25°C, antioxidant activity decreased between the first and second week. The berries coated with 3% chia oil had higher antioxidant activity values compared to those not coated with chia. These results suggest that the incorporation of 3% chia oil into the chitosan coating helps maintain or enhance the antioxidant capacity of berries during storage, making this formulation a promising strategy for preservation through functional biopolymeric coatings.

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Synthesis of Two New Indole-Derived Pyrazolopyrimidines: Characterization and Antituberculosis Activity

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In the present work, is integrated the synthesis, structural and supramolecular characterization, antimicrobial activity assays, molecular docking and DFT analysis for 2-(1-hexyl-1H-indol-3-yl)-5,7-dimethylpyrazolo[1,5-a]pyrimidine (Hexa) and 5,7-dimethyl-2-(1-octyl-1H-indol-3-yl)pyrazolo[1,5-a]pyrimidine (Octa) novel compounds. The results of antibacterial activity on clinically relevant mycobacteria show that just Oct compound shows potential activity on all species of mycobacterium at a concentration of 256 µg/ml. The experimental results were corroborated by DFT and molecular docking analyses, where Octa binds Mycobacterium tuberculosis targets more strongly than Hexa, favoring deep, stabilizing hydrophobic and π–stacking interactions. These results show that the new molecules can be considered as potential drugs for the control of tuberculosis [1]

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Synthesis of New Azo-Azomethine-Imino Pyrazole Derivatives: Characterization and Antifungal Activity

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Pyrazole derivatives of Schiff bases containing azo-azomethine-imino pyrazoles were synthesised in order to ascertain the impact of introducing substituents, such as chlorine and the methoxy group, to the aromatic ring. The unsubstituted pyrazole derivative exhibited moderate biological activity [1]. The pyrazole Schiff base derivatives were characterised using elemental analysis, IR, NMR, UV-Vis, XRD and DFT. The experimental data agree very well with those obtained using density functional theory (DFT). The results from single-crystal X-ray diffraction showed that the two pyrazolyl derivatives of azoazomethine adopt conformations stabilized by a strong intramolecular O–H···N hydrogen bond. Replacing chlorine with a methoxy group results in a flatter molecular geometry, a decrease in the HOMO and LUMO energy gaps, and, in UV-Vis spectroscopy, a bathochromic shift of the lower-energy electronic transition. Biological evaluation against C. albicans and C. neoformans revealed that both derivatives exhibit limited antifungal activity, indicating that the observed differences in molecular flatness and electronic properties do not translate into improved biological performance compared to the previously published unsubstituted compound AZO3 [2].

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EFFECT OF COMPOSITION AND DRYING TEMPERATURE ON THE INTERFACIAL BEHAVIOR OF ACYLATED AGAVE FRUCTAN–CHITOSAN COMPLEXES IN PICKERING W/O/W EMULSIONS

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Water-in-oil-in-water (W/O/W) emulsions are promising carriers for hydrophilic bioactive compounds, although their physical stability remains challenging because of the presence of two interfaces [1,2]. Bio-based Pickering particles offer an alternative strategy to reinforce these interfaces and improve multiple-emulsion stability [1,2]. This study evaluated the effect of composition and drying temperature on the wettability and interfacial behavior of acylated agave fructan–chitosan complexes and their performance in Pickering W/O/W emulsions. Acylated agave fructan (FNA) and chitosan (QUIT) were complexed at FNA:QUIT ratios of 1:1 and 1.2:1, and the insoluble fractions were dried at 50 or 60 °C. Apparent oil contact angle and dynamic interfacial tension (IFT) at the canola oil–water interface were determined, while droplet-size evolution was monitored by optical microscopy over 30 days. Apparent oil contact angles ranged from 66.98 to 101.45°, indicating composition- and drying-dependent differences in wettability, a key factor in particle attachment and Pickering stabilization [3]. All formulations showed a time-dependent decrease in IFT. At 20 min, complexes dried at 60 °C exhibited lower IFT than their 50 °C counterparts: 4.50 versus 9.69 mN m^{-1} for the 1:1 ratio and 9.32 versus 12.90 mN m^{-1} for the 1.2:1 ratio, indicating faster interfacial adsorption at the higher drying temperature. This interpretation is consistent with experimental evidence that adsorption of particles at fluid interfaces decreases the apparent interfacial tension through interfacial area replacement [4]. Among the evaluated systems, the 1:1 complex dried at 60 °C showed the lowest relative variation in Sauter mean diameter ($D_{3,2}$), from 36.74 to 39.26 µm over 30 days (+6.9%). Overall, the results indicate that complex composition and drying temperature modulate particle wettability, interfacial adsorption kinetics, and droplet-size evolution in Pickering W/O/W emulsions. These findings provide a physicochemical basis for selecting formulation conditions for the development of bio-based multiple-emulsion delivery systems.

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Optimization of alginate–chitosan hydrogels through ionic crosslinking for advanced wound dressing applications

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This work presents the design and development of alginate–chitosan-based hydrogels for skin wound healing applications [1]. The proposed system incorporates silver nanoparticles and graphene into the polymeric network to combine their physicochemical, mechanical, and antibacterial properties in a multifunctional material [2,3].

The hydrogel formulation was designed by varying the alginate-to-chitosan ratio and sodium tripolyphosphate (TPP) concentration as an ionic crosslinker. At the current stage, swelling behavior was evaluated in phosphate-buffered saline (PBS, pH 7.2) over 72 h to identify the most suitable formulations. All hydrogels exhibited rapid initial water uptake followed by a slower increase without reaching equilibrium. Swelling capacity strongly depended on polymer ratio and TPP concentration. Hydrogels with a 1:1 ratio showed the highest swelling at low crosslinking (above 400% at 72 h) but greater variability and lower structural stability at higher TPP concentrations. In contrast, 2:1 systems displayed more homogeneous swelling (≈195–253%), suggesting a more compact network. 3:1 hydrogels showed the best balance between absorption and reproducibility (≈250–350%) while maintaining structural integrity. Overall, 35 mM TPP provided the best balance of swelling, stability, and reproducibility, particularly for the 2:1 and 3:1 formulations. Selected hydrogels will be characterized by scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR) before and after swelling, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and rheology. Graphene and silver nanoparticles will then be incorporated into the optimized systems, and the same analyses will assess their effects on the structural, thermal, and mechanical properties.

This approach will provide insight into the relationship between polymer composition, crosslinking conditions, and hydrogel performance. Ultimately, the developed system aims to provide structural stability, moisture retention, and potential antibacterial activity for wound healing applications.

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pH-sensitive PVA comb-like hydrogels with methacrylamide and acrylic acid obtained by gamma radiation for drug release

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Aqueous solutions of poly(vinyl alcohol) (PVA) with molecular weights of 99,000 and 31,000 g/mol at different concentrations were irradiated with gamma rays from a ^{60}Co source to obtain *net*-PVA hydrogels [1]. In this first step, the influence of PVA molecular weight on the crosslinking reaction was studied [2] by varying the dose. The second step was the simultaneous grafting of methacrylamide (MAAm) and acrylic acid (AAc) to obtain comb-like hydrogels. In this case, the MAAm monomer concentration, solvent, and dose were studied. In its polymeric form, AAc exhibits a response to pH, giving this property to the material in which it is grafted; therefore, (*net*-PVA)-*g*-MAAm/AAc hydrogels have a pH response. PVA hydrogels and the grafted ones were characterized using various techniques: infrared spectroscopy (FTIR-ATR), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM). Its physicochemical properties were also studied through limit swelling tests in water, reaching 4000%; determination of the critical pH (pH = 5.0); and swelling in phosphate buffer, simulating a physiological fluid, reaching around 3000%. Finally, the loading and release kinetics of an antiseptic (benzalkonium chloride) in comb-like hydrogels were studied, showing sustained release over 24 hours and fitting a Peppas-Sahlin release model. Therefore, this material is expected to have potential applications in wound treatment [3].

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HYBRID NANOMATERIALS FOR THE TREATMENT OF RHEUMATOID ARTHRITIS

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Rheumatoid arthritis (RA) affects up to 1.2% of the population in Mexico and is associated with a high cardiovascular risk, where arterial stiffness is an early indicator [1]. Drugs such as enalapril and methotrexate help control these complications, but their combined administration results in low adherence to treatment due to multiple drug interactions [2]. To overcome these challenges, a smart delivery system is proposed based on mesoporous silica nanoparticles (MCM-41) combined with biopolymers such as chitosan or cyclodextrin, which provide high loading capacity and biocompatibility. MCM-41 was synthesized by a sol-gel method and characterized by FTIR, SEM, BET surface area, among others. SEM images showed slightly elongated particles (100-120 nm) (**Fig.1a**), with uniform sizes and a homogeneous distribution (**Fig.1b**), confirming the nanometric dimension. Finally, the preliminary evaluation of MTX (methotrexate) loading capacity demonstrated a capacity of 40% without reaching saturation of the nanomaterial (**Fig.1c**).

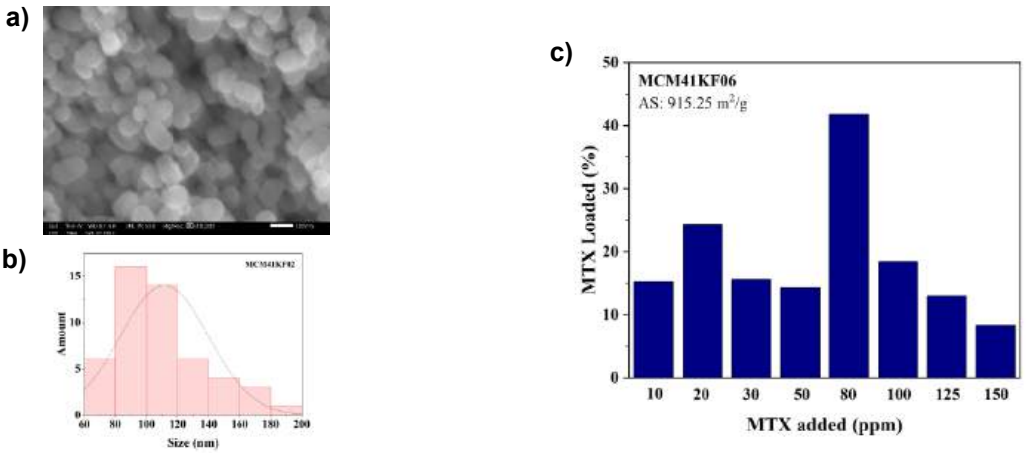

Figure 1. a) SEM microscopy of a mesoporous silica sample, b) distribution obtained from the sizes analyze in the microscopy. c) Load capacity study.

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Abstract preparation

Upcycling Post-Consumer Polystyrene into a Zirconium-Functionalized Hybrid Adsorbent for Fluoride Removal

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Post-consumer polystyrene is a persistent polymeric waste whose chemical stability limits its natural degradation and promotes its accumulation in the environment. Its conversion into functional materials represents a promising strategy for waste valorization and the development of sustainable technologies for water treatment. This study aimed to prepare a zirconium-functionalized hybrid adsorbent from post-consumer polystyrene and evaluate its performance for fluoride removal from aqueous solutions. The polymer was cleaned and subjected to a surface pretreatment, followed by sulfonation to introduce functional groups capable of anchoring zirconium-containing species. FTIR analysis showed that the modified material retained the characteristic aromatic structure of polystyrene, as evidenced by the C–H stretching band at 3029 cm^{-1}. A broad band centered at 3380 cm^{-1} was associated with O–H groups from sulfonic functionalities and adsorbed water. The bands at 1172, 1122, and 1004 cm^{-1} were attributed to S=O and S–O vibrations, supporting successful sulfonation. Furthermore, the low-wavenumber bands observed at 620 and 541 cm^{-1} were consistent with Zr–O and potentially Zr–O–S vibrations, supporting the interaction of zirconium-containing species with the sulfonated polymer matrix. Fluoride adsorption was evaluated at pH 3, an initial fluoride concentration of 5 mg/L, a contact time of 60 min, and an adsorbent dosage of 1 g/L. Under these conditions, the material decreased the fluoride concentration from approximately 5 to 1 mg/L, corresponding to nearly 80% removal and an estimated adsorption capacity of 4 mg/g. These results indicate that post-consumer polystyrene can be transformed into a zirconium-functionalized hybrid material with potential application in fluoride-contaminated water treatment, integrating polymer waste upcycling, sustainable materials development, and environmental remediation within a circular-economy framework.

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A new generation of pyrene based tripods for facilitated interfacing of graphene with biomolecules

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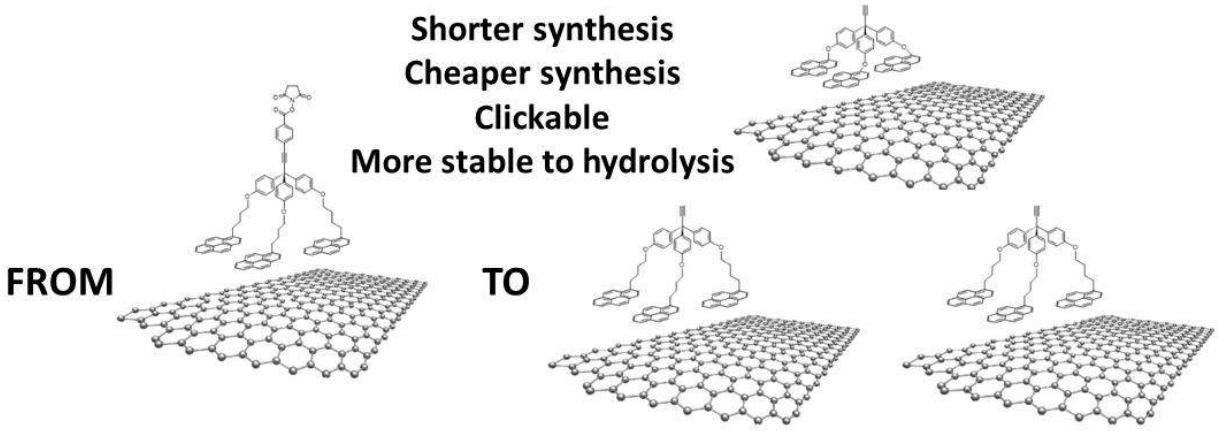
Abstract-
Graphene's exceptional properties such as high surface to volume ratio, electrical conductivity, transparency and mechanical strength make it a promising material for various bio-based applications. However, its inherent hydrophobicity limits interactions with biomolecules, since they can undergo conformational changes and loose their function when placed in close proximity of the surface. While conventional monofunctional linkers (e.g., PBASE) have been widely used, tripodal molecules offer superior stability and biomolecule immobilization efficiency, particularly for antibodies and nanobodies. In this work, we introduce a new generation of tripodal compounds that addresses key challenges that have limited their adoption by the graphene community: cost, ease of preparation, sensitivity to hydrolysis. Our approach incorporates alkynes to enable streamlined functionalization via CuAAC click chemistry, thereby optimizing both synthetic accessibility and sensor performance while increasing versatility. The functionalization of graphene for biosensing using this new generation of tripods has been monitored by quartz crystal microbalance with dissipation monitoring (QCM-D) enabling exhaustive quantitative characterization of each step of the functionalization protocol. This innovative tripod based functionalization protocol was consecutively applied to the surface of graphene-based solution-gated field-effect transistors (SGFET) effectively turning them into real time biosensors. Such biosensors sensing performances were tested again *Escherichia Coli* bacterial target to forecast the potential of this technology in environmental monitoring and sanitary surveillance of waters.



ARTIFICIAL NEURAL NETWORKS FOR PREDICTING DRUG ADSORPTION: THE CASE OF NAPROXEN ON MIL-101

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The continuous use of over-the-counter pharmaceuticals such as naproxen has led to their widespread presence in the environment, specifically in natural water bodies and wastewater treatment plants [1]. Despite occurring at very low concentrations (µg/L), conventional treatment methods have proven insufficient for their complete removal, and their persistence in aquatic ecosystems poses a significant threat to aquatic organisms and the environment [2].Emerging contaminants like naproxen can be efficiently removed from water using adsorbent materials such as metal-organic frameworks (MOFs). This work proposes the application of artificial neural networks (ANNs) to predict the adsorption capacity of this drug onto MIL-101. The dataset was obtained from the literature, specifically from the paper “Adsorptive removal of naproxen and clofibric acid from water using metal-organic frameworks” [3], which explores various factors influencing adsorption, including contact time, initial contaminant concentration, and pH. The developed ANN features a 3:10:1 architecture and was trained using the ReLU activation function. Model performance was evaluated using the correlation coefficient (R^2 = 0.98). The predicted optimal conditions for naproxen adsorption onto MIL-101 were a pH of 4.5, an initial naproxen concentration of 15 ppm, and a contact time of 5 h.

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Molecular Design of BODIPY–Steroid Derivatives for Viscosity-Sensitive Theranostic Platforms

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Boron-dipyrromethene (BODIPY) dyes are attractive chromophores for functional materials and biophotonic systems owing to their intense absorption, sharp emission, and tunable photophysical behavior through substitution at multiple positions of the dipyrromethene core [1]. Conjugation of BODIPY scaffolds with biologically relevant fragments is a rational strategy toward multifunctional platforms combining an optical readout with the features of the appended unit.

In this work, a BODIPY core was coupled under Sonogashira conditions with alkynyl-steroid derivatives of norethisterone and etisterone, and the resulting conjugates were further brominated at the 2- and 5-positions to give the corresponding dibrominated analogues. All products were characterized by NMR spectroscopy.

The photophysical response of the BODIPY–norethisterone conjugate to microviscosity was evaluated by UV-Vis and fluorescence spectroscopy in DMSO/glycerol mixtures. Fluorescence intensity increased markedly with the glycerol proportion while the emission maximum remained essentially unchanged, consistent with a viscosity-driven modulation of non-radiative decay. Analysis using the Förster–Hoffmann relation [3], characteristic of molecular-rotor-type fluorophores [2], yielded a slope of m = 0.6227 (R^2 = 0.9986). A similar response was observed for the brominated conjugate and the etisterone-based analogue, supporting the generality of this behavior within the series.

These results indicate that BODIPY–steroid conjugates are a synthetically accessible family of fluorophores sensitive to the microviscosity of the surrounding medium, of interest for molecular platforms potentially useful for theranostic applications. Ongoing work targets their singlet-oxygen-generating ability.

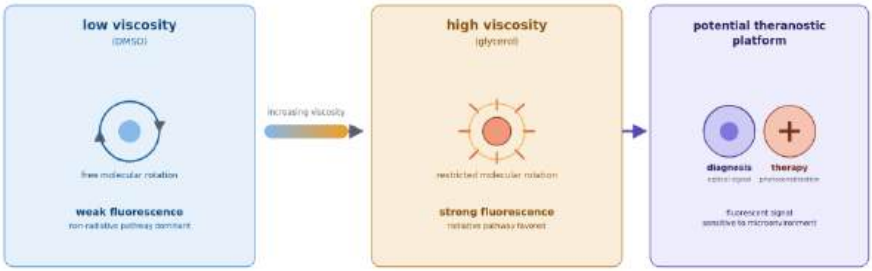

Figure 1. Conceptual illustration of the viscosity-sensing behavior and potential theranostic platform based on BODIPY–steroid conjugates.

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Sustainable Valorization of Tejocote (*Crataegus* spp.) through Pectin Extraction and Structural Characterization

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Tejocote (*Crataegus* spp.) is a native Mexican fruit with a naturally high pectin content and a limited range of industrial applications beyond seasonal food products. Its valorization as a renewable source of bio-based polymers may contribute to the sustainable utilization of this underexplored fruit resource. In this study, pectin was extracted from tejocote fruits using acid-assisted and ultrasound-assisted extraction and subsequently characterized through complementary physicochemical and spectroscopic approaches. Acid-assisted extraction was performed at pH 1.6 and 84 °C for 1 h, whereas ultrasound-assisted extraction was conducted at pH 2.0, 70 °C, 200 W, and 40 kHz for 30 min. Pectin yields of 29.07 ± 0.74% and 29.24 ± 0.43% were obtained for acid-assisted and ultrasound-assisted extraction, respectively, with no statistically significant difference between the methods (p = 0.785). The extracted pectin exhibited a degree of esterification of 36.09 ± 0.61%, corresponding to a low-methoxyl pectin, and an anhydrouronic acid content of 29.94 ± 0.26%. ATR-FTIR analysis revealed the characteristic functional groups of pectin, including esterified and non-esterified carboxyl groups, while solid-state ^13C CP/MAS NMR provided complementary information on the polysaccharide structure. Characteristic resonances associated with carbonyl, anomeric, methoxyl, and acetyl carbons were identified. The degree of methylation estimated by ATR-FTIR and solid-state ^{13}C CP/MAS NMR was 45.37% and 55.87%, respectively. The results demonstrate that tejocote can serve as a promising renewable source of low-methoxyl pectin and highlight the value of complementary spectroscopic techniques for establishing structural characteristics. This work contributes to the development of value-added bio-based materials from underutilized Mexican fruit resources.

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Smart Gatekeepers: pH-Responsive Silica Hybrids for Controlled 5-Fluorouracil Release

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Stimuli-responsive polymeric shells can transform mesoporous silica nanoparticles (MSNs) into molecular gatekeepers capable of regulating drug accessibility in response to acidic environments [1-3]. However, establishing a direct relationship between their functional performance and their dynamic, hydrated architecture remains a critical challenge [3,4]. In this work, we engineered pH-responsive ellipsoidal MSNs for the pH-responsive delivery of the anticancer drug 5-fluorouracil (5FU). The nanoparticles were functionalized with a poly(DEAEMA-co-HEMA) shell via an aqueous “grafting-from” strategy, exploiting the pH-dependent swelling of PDEAEMA (pKa ≈ 6.9) together with the stabilizing and biocompatible character of PHEMA [4].
Conventional characterization techniques (FTIR, XPS, TEM/SEM, and TGA) confirmed successful surface modification, revealing uniform ~120 nm core–shell nanoparticles with grafting yields of up to 60%. To resolve their three-dimensional organization in the hydrated state, small-angle neutron scattering (SANS) with silica-core contrast matching (~58% D_2O) was employed. Under strongly acidic conditions (pH 2), SANS revealed that the hydrated polymer shells adopt a substantially more extended and anisotropic configuration than suggested by dry-state characterization. This solution-state structural insight provides a critical basis for understanding the pH-dependent behavior of these hybrid gatekeepers. The resulting nanocarriers exhibited a maximum 5FU loading efficiency of 26% ± 4%, demonstrating their potential as pH-responsive platforms for controlled drug delivery.

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EFFECT OF CELLULOSE MODIFICATION ON THE PERFORMANCE OF APP-BASED INTUMESCENT POLYPROPYLENE COMPOSITES

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Intumescent flame-retardant (IFR) systems represent an effective halogen-free strategy for improving polymer fire safety through the formation of protective carbonaceous layers during combustion. In this work, microcrystalline cellulose was sequentially functionalized by cyanoethylation and subsequent tetrazole formation to transform a renewable carbon source into a nitrogen-rich functional component capable of enhancing phosphorus–nitrogen interactions in polypropylene (PP)-based intumescent systems. Successful cellulose functionalization was confirmed by FTIR and NMR spectroscopy. The resulting cellulose derivatives were incorporated into PP, either individually or in combination with ammonium polyphosphate (APP), by melt blending. The thermal stability, fire behavior, mechanical performance, and morphology of the combustion residues were systematically investigated by thermogravimetric analysis (TGA), cone calorimetry, horizontal UL-94 testing, tensile measurements, and scanning electron microscopy (SEM). Although the modified celluloses alone produced only moderate improvements in flame-retardant performance, their combination with APP resulted in a pronounced synergistic effect. In particular, tetrazole-functionalized cellulose exhibited the strongest interaction with APP, producing the lowest peak heat release rate (PHRR) of 899 kW m^{-2}, corresponding to a 39% reduction relative to neat PP and also promoting the formation of a compact, phosphorus-rich carbonaceous residue. The resulting protective structure enhanced condensed-phase activity and limited heat and mass transfer during combustion. These results demonstrate that introducing nitrogen-rich tetrazole groups into cellulose provides an effective molecular strategy for converting a conventional bio-based carbon source into an active component of phosphorus–nitrogen intumescent systems. This approach offers a promising pathway toward more efficient and sustainable halogen-free flame-retardant PP composites.

Keywords: polypropylene; intumescent flame retardancy; cellulose; tetrazole; ammonium polyphosphate; phosphorus–nitrogen synergy; bio-based flame retardants.

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NOVEL THERMOSTABLE THERMOSETTING FILMS AND FOAMS

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Thermostable polymer matrices are widely used in aerospace industry and microelectronics. Among them, thermosetting benzoxazines (BOAs) and cyanate ester resins (CERs) expand the high-temperature operation regime, thus constituting the most promising materials. It is well known that the benzoxazine ring is stable at low temperature, but a ring opening reaction occurs at high temperature, and novolac type oligomers having both phenolic hydroxyl group and tertiary amine group are produced. Polybenzoxazines (PBZs), a new type of phenolic resin that releases no volatiles during curing reaction and needs no catalysts is thus developed. Benzoxazine monomers exhibit many other attractive properties, such as low melt viscosity. In addition, the polymer is characterized by low volumetric shrinkage upon polymerization, low moisture absorption, excellent chemical resistance, flame retardancy, electrical properties, thermal stability, mechanical properties; and very rich molecular design flexibility [1]. On the other hand, CERs differ from others by a very regular structure of the resulting polymer networks, namely polycyanurates (PCNs), obtained by their polycyclotrimerization. They have received much attention because of their unique combination of physical properties, including high thermal stability (> 400°C), high glass transition temperature (> 270°C), high fire-, radiation and chemical resistance, low water absorption and low outgassing, high adhesion to different substrates, and excellent dielectric properties (ε = 2.6−3.1). As a result, CERs are currently used as structural or functional materials in aeronautics, printed circuit boards or adhesives [2,3].

In this lecture, we address the copolymerization of CERs and BOAs by FTIR and DSC in order to get an insight into the structure and properties of resulting hybrid thermosets based on PCNs and PBZs. Novel POSS-containing nanocomposites derived from such hybrid thermosets are developed. Novel insights into several pore generation approaches to (nano)porous PCN materials, including films and foams, are also given [4]. The combination of low thermal conductivity, low thermal diffusivity, and relatively high specific heat capacity makes PCN foams promising candidates for thermal insulation applications.

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Energy recovery from water hyacinth using an integrated modular system for anaerobic digestion and biogas enrichment for biomethane production

Presenting Guillén Pérez María Fernanda[1], Hernández Aguilar Adrián[2], Romero Cruz Marco[3], Torres Sandoval Indira[4], Mena Cervantes Violeta Yasmin[5*], Aguilar Aguilar Fidel Alejandro[6*]

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Water hyacinth (*Eichhornia crassipes*) is an invasive aquatic species that has covered approximately 87–88% of the surface of the Zumpango Lagoon in Mexico, causing ecological degradation and generating large amounts of residual biomass [1]. This study evaluates its energy potential and proposes an integrated modular system for converting the harvested biomass into biomethane within a circular economy framework. The physicochemical properties of floating petioles, leaves, petioles, roots, rhizomes, and the whole plant were determined by measuring moisture, total solids (TS), volatile solids (VS), ash, and C/N ratio [2]. Biochemical methane potential tests were conducted in batch reactors, and the composition of the resulting biogas was experimentally quantified. The whole plant exhibited a moisture content of 88.66%, TS of 11.34%, VS of 9.63% on a wet basis, a VS/TS ratio of 0.849, and a C/N ratio of 22.77. It produced 374.07 NmL of biogas per g VS, with a methane concentration of 59.67% and an experimental methane yield of 223.21 NmL CH_4/g VS. Compared with its theoretical methane potential of 267.97 NmL CH_4/g VS, the whole plant achieved a biodegradability of 83.29%, indicating that separation of the biomass into individual plant fractions may not be required before anaerobic digestion. Based on these results, a pilot-scale modular configuration with a nominal capacity of 1 m³ is proposed, integrating wet biomass size reduction, anaerobic digestion, biogas upgrading, gas storage, and process monitoring. For an 800 L working volume and an organic loading rate of 2 kg VS/m³·d, the system could process approximately 16.6 kg of fresh biomass per day and generate an estimated 0.60 m³ of biogas or 0.36 m³ of methane per day, equivalent to approximately 3.56 kWh/d of chemical energy. A dual fixed-bed upgrading stage is proposed to sequentially remove H_2S and CO_2 and increase the methane concentration to biomethane-quality levels. This integrated approach supports circular economy and climate-change mitigation strategies by simultaneously addressing an invasive aquatic biomass, reducing its environmental impact, and producing a decentralized renewable fuel that could contribute to the environmental recovery of the Zumpango Lagoon.

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Fluorescence spectroscopy for monitoring the structural stability and release of insulin glargine encapsulated in Poloxamer 407

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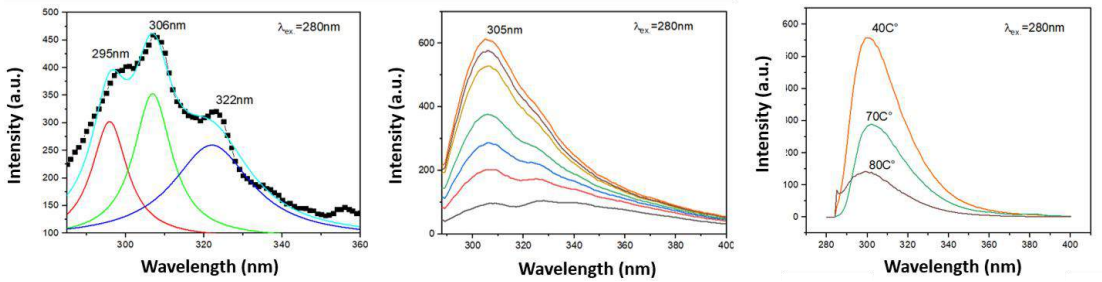
Diabetes mellitus requires drug delivery systems capable of improving glycemic control while preserving insulin stability. In this work, Poloxamer 407 (Pluronic® F127) was evaluated as a thermosensitive carrier for insulin glargine encapsulation [1]. Formulations containing different insulin concentrations were prepared, freeze-dried, and characterized by UV–Vis, FTIR and fluorescence spectroscopy. UV–Vis spectra revealed a characteristic absorption band of insulin at 275 nm. FTIR analysis revealed bands associated with α-helical (~1658 cm^{-1}) and β-sheet (1615–1640 cm^{-1}) structures, suggesting preservation of the characteristic secondary structure of insulin after encapsulation. Insulin release was evaluated at pH 4 for 90 min using intrinsic fluorescence spectroscopy. Excitation at 280 and 275 nm produced emission maxima at 305 and 304 nm, respectively, with no significant spectral shifts during the release assay, indicating that the local environment of aromatic residues remained essentially unchanged. These findings suggest that Poloxamer 407 preserves the structural integrity of insulin glargine during encapsulation and that fluorescence spectroscopy provides a suitable, non-destructive approach for monitoring its release [2,3].



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Correlations Properties in Functional hybrid MoOx-PEDOT:PSS on Flexible Substrates for PEC´s

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The transition toward sustainable energy solutions relies heavily on the development of high-performance functional polymers and organic materials for energy applications. In this work, we present the fabrication and characterization of a solid-state photoelectrochemical cell (PEC) architecture utilizing a hybrid functional MoOx-PEDOT:PSS polymeric active layer that have shown excelent eletronic properties [1]. To address the environmental impact of synthetic polymers, these hybrid functional films were grown on both traditional poly(ethylene terephthalate) (PET) and renewable, bio-based dried palm leaf substrates. We evaluate the structure-property-performance correlations, focusing on how the synergistic effects between the MoOx and the functional organic matrix enhance the work function and charge transportation capacity. Furthermore, optical characterization revealed significant structure-related emission properties. The fluorescence response of the MoOx-PEDOT:PSS film deposited on PET shows emission features centred at approximately 420, 440, 490 and 530 nm. While the intense bands at 320 and 360 nm were not considered for chemical assignment because they may include scattering-related contributions in the excitation–emission matrix, the 420–440 nm region is consistent with the intrinsic blue fluorescence of PET. In contrast, the bands at 490 and 530 nm are more consistent with defect-related emission from MoOx, particularly oxygen-vacancy and deep-defect states, and are therefore the most representative features of the oxide contribution in the functional films. By integrating functional organic materials with sustainable substrates, this study provides critical insights into interface optimization for next-generation sustainable flexible organic energy applications.

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Development and Evaluation of Copper Gluconate-Loaded PLGA Particles

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Copper is an essential trace element, and alterations in its homeostasis have been associated with diseases related to copper metabolism, such as Menkes disease and amyotrophic lateral sclerosis (ALS) [1, 2]. However, conventional administration is limited by bioavailability, non-specific biodistribution, and potential toxicity resulting from bioaccumulation and elevated concentrations in unintended tissues [3]. Copper gluconate is one of the salts used as a source of copper supplementation. In this context, polymeric modified-release systems offer a strategy to promote the gradual delivery and stability of the metal while supporting safer therapeutic profiles [4]. Poly(lactic-co-glycolic acid) (PLGA) is a synthetic, biodegradable, and biocompatible polymer widely used in drug delivery systems (DDS) [5]. The aim of this study was to develop and evaluate a polymeric system based on PLGA microparticles and nanoparticles loaded with copper gluconate as an alternative for the modified delivery of this trace element. To this end, particles were produced using double emulsion (W/O/W) and nanoprecipitation techniques, employing polyvinyl alcohol (PVA), poloxamer 407, and polysorbate 80 as stabilizers. The microparticles had a mean size of 2.05 µm, while the nanoparticles had an approximate size of 140 nm; both exhibited a spherical morphology, as observed by optical microscopy and scanning electron microscopy (SEM). Thermogravimetric analysis (TGA) was used to evaluate the system's thermal stability and evidenced solvent removal, while Fourier-transform infrared spectroscopy (FTIR) showed that the encapsulation process caused no appreciable chemical changes in the components. Furthermore, release studies demonstrated a profile consistent with modified release. These results demonstrate the feasibility of producing copper gluconate-loaded PLGA particles with potential application as a DDS for the prolonged delivery of this trace element.

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Graphene Supramolecular Frameworks.

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A novel category of frameworks was developped by implementing graphene grafted at the periphery with Ni-Salphen complexes as hybrid building blocks, while employing $[PdCl_2(PTA)_2]$ (PTA= 3,5,7-triaza-7-phosphaadamantane) complexes as ditopic linkers. Graphene Supramolecular Frameworks (GSFs) were formed, differing themselves by the grafting angle of the Ni-Salphen hinges on the graphene based building blocks. GSFs were fully characterized by IR spectroscopy, PXRD, TGA, DSC, SEM-EDS and XPS.

Spectrophotometric supramolecular titrations were performed to validate the affinity of the selected building blocks to reticulate, by first evaluating the capability of the $[PdCl_2(PTA)_2]$ complex to perform as a ditopic linker to the Ni-Salphen complexes, confirming a 1:2 $[PdCl_2(PTA)_2]$:Ni-Salphen binding stoichiometry. XPS studies on the interaction of the grafted [Ni] binding site with the linker revealed the concatenation of the species, that alongside fluorescence enhancement dependent on linker's concentration and Hill's analyses, demonstrated a cooperative supramolecular oligomerization processes.

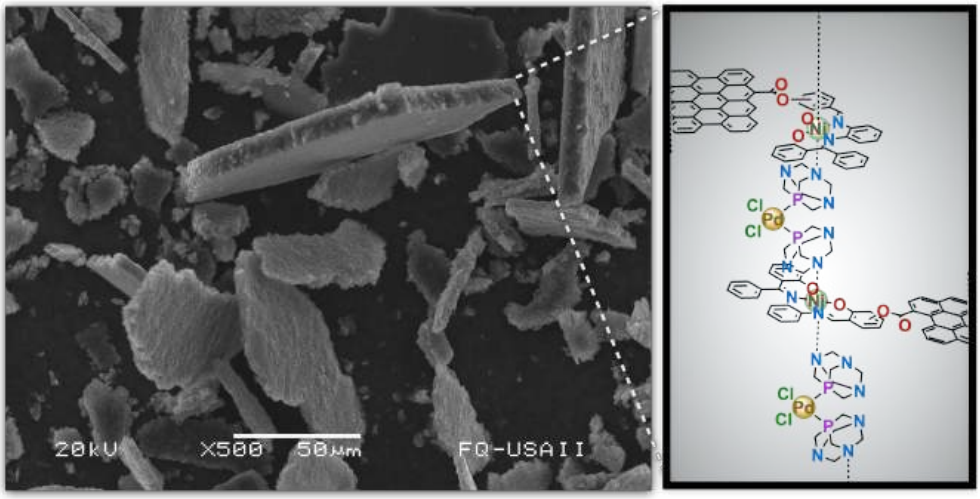

Figure 1. SEM microgograph of a GSF and a representation of it's composition.

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Abstract preparation

Design and fabrication of an inertial system for the removal of microplastics

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Microplastic (MP) pollution poses a growing threat to aquatic ecosystems and human health due to its persistence, bioaccumulation, and the difficulty of removing it using conventional water treatment systems. In this context, the objective of this research is to design and manufacture an inertial system for the removal of microplastics. To this end, a test bench was designed, manufactured, and put into operation to simulate real-world water transport conditions, enabling the analysis of the inertial system in terms of microplastic removal, head loss, and hydraulic efficiency. The designed prototype complies with international standards, and preliminary results demonstrate its ability to evaluate MP removal and its impact on the hydraulic system. This study seeks to contribute to the development of sustainable solutions for improving water quality through filtration technologies applicable to the operation of pumping systems.

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TWENTY-FIVE YEARS OF RESEARCH ON SELF-ASSEMBLY, PHASE BEHAVIOR AND MICELLAR DYNAMICS OF PEO–PPO BLOCK COPOLYMERS IN AQUEOUS MEDIA

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Amphiphilic block copolymers based on poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO), including Pluronic® (PEO–PPO–PEO) and reverse Pluronic® (PPO–PEO–PPO) architectures, are widely used model systems for studying self-assembly in soft matter. In aqueous media, these materials exhibit a rich phase behavior that spans from dilute micellar solutions to ordered liquid-crystalline phases and gel-like networks, governed by molecular architecture, concentration, and temperature.

Over more than two decades, the Rheology Laboratory at the University of Guadalajara has systematically investigated the phase behavior, structure, and dynamics of representative systems such as L64, P84, P103, P104, F108, and F127. Through the combined use of rheology, light scattering, microscopy, and calorimetry, detailed phase diagrams have been established and the mechanisms of micellization, micellar growth, and ordering transitions have been elucidated [1–3].

A central focus of these studies has been the coupling between equilibrium structure and dynamic behavior. In particular, micellar exchange processes, viscoelastic relaxation, and thermally induced structural transitions have been analyzed to establish relationships between nanoscale dynamics and macroscopic rheological response [2,3]. These results have contributed to a deeper understanding of transient network formation and the emergence of complex fluid behavior in amphiphilic block copolymer systems.

This contribution summarizes key findings from a long-term collaborative research effort led by J. Félix Armando Soltero Martínez and co-workers, highlighting the role of Pluronic and reverse Pluronic systems as model advanced materials for exploring self-assembly, phase transitions, and dynamic processes in soft condensed matter [1–4].

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Biocompatible PCL-Hidroxyapatite/Silica composites as controlled drug delivery systems for ibuprofen and tramadol

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Pain is a global public health problem that significantly affects quality of life. Conventional treatments for this condition are associates with various adverse effects and low therapeutic efficiency. Therefore, controlled and localized drug deliveery systems represents a promising alternative to improve pain management and reduce side effects. Ibuprofen, a nonsteroideal antiinflammatory drug, and tramadol, an analgesic, present limitations associated with their conventional administration, which highlights the need for alternative drug delivery approaches. The aim of this study was to evaluate the potential of polymer-ceramic composites for controlled and localized drug delivery. Hidroxyapatite and silica were evaluated as ceramic reservoirs for the delivery of ibuprofen and tramadol and polymer-ceramic composites were developed using polycaprolactone (PCL) as the polymeric matrix with potential application in transdermal drug delivery systems. The obtained materials were characterized using different analytical techniques. Scanning electron microscopy (SEM) analysis revealed differences in the morphology of the materials, while X-ray diffraction (XRD) results confirmed the corresponding crystalline phases. The presence of characteristic functional groups of PCL and the loaded drugs were confirmed by Fourier transform infrared spectroscopy (FTIR). Drug adsorption and release were evaluated by UV-Vis spectroscopy, showing different release profiles depending on the ceramic material an its incorporation into the polymeric matrix. These results suggest that the composition and structure of the materials influence sustained drug release behavior.

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FROM PLANT BIOMASS AND WASTE TO FUNCTIONAL MATERIALS: SUSTAINABLE MODIFICATION OF POLYMERIC, CEMENTITIOUS, AND ASPHALT SYSTEMS

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The increasing generation of agroindustrial and textile wastes represents both an environmental challenge and an opportunity to produce value-added materials. In Mexico, the tequila industry generates approximately 750,000 tons of *Agave tequilana* bagasse annually, while nopal production generates nearly 300,000 tons of residual cladodes. Globally, around 92 million tons of textile waste are produced each year. Other lignocellulosic resources, such as *Acacia farnesiana* (Huizache), remain underutilized because its shrubby anatomy limits its wood applications mainly to fences and small products. These resources offer significant potential for developing functional bio-based materials within a circular-economy framework. Different processing routes were explored depending on the biomass source and intended application. Cellulose isolated from *Agave tequilana* bagasse[1], Huizache[2], and cotton-rich post-consumer denim was processed to obtain cellulose nanocrystals (CNCs)[3]. Agave bagasse was also converted into cellulose pulp as a less processing-intensive alternative for applications requiring larger material volumes[4]. Additionally, mucilage, a polysaccharide-rich biopolymer, was extracted from residual *Opuntia velutina* cladodes for use in cementitious materials[5]. The resulting bio-based materials were incorporated into matrices with different physicochemical characteristics. In acrylic acid/acrylamide hydrogels, CNCs modified swelling and mechanical properties[2,6]. In Portland cement mortars and PLA composites at low CNC concentrations substantially improved mechanical performance[1]. Agave-derived CNCs also modified asphalt rheological behavior[7], while agave cellulose pulp was explored as a more economically feasible alternative and enhanced the performance of Stone Mastic Asphalt[4]. *Opuntia velutina* mucilage improved cementitious materials and showed potential as a natural corrosion inhibitor in reinforced concrete[5]. Overall, these studies demonstrate that wastes and underutilized biomass can be transformed into functional materials at different structural scales and for diverse engineering applications. The materials of the future may increasingly originate from our own wastes, transforming environmental liabilities into technological resources and contributing to sustainable materials development within a circular economy.

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CHITIN AND CHITOSAN FROM BLACK SOLDIER FLY: SUSTAINABLE BIOMATERIALS FOR COSMETIC APPLICATIONS

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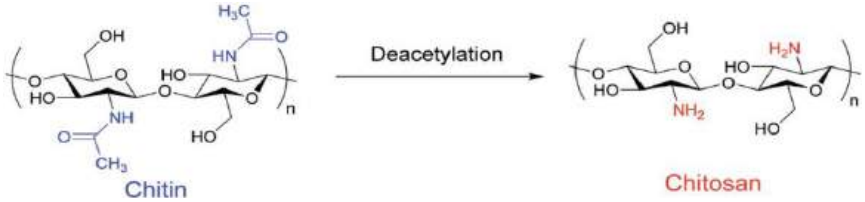
The rapid expansion of the insect bioconversion industry has created new opportunities for the sustainable valorization of insect-derived by-products within the framework of the European circular bioeconomy. Among these, the Black Soldier Fly (BSF) has emerged as an efficient bioconverter of organic waste, producing proteins, lipids, and frass for diverse industrial applications. However, pupal exuviae remain an underutilized by-product despite their high chitin content.

This work explores sustainable strategies to valorize BSF pupal exuviae into chitin and high-value chitosan for cosmetic applications, contributing to resource efficiency and waste reduction [1]. Chitin extraction is performed through an environmentally friendly process involving defatting, milling, demineralization, deproteinization, bleaching, and purification. Subsequent deacetylation produces chitosan with controlled molecular weight and degree of deacetylation, enabling the tailoring of its physicochemical properties for cosmetic formulations.



Compared with conventional crustacean-derived chitosan, BSF provides a sustainable and traceable alternative through year-round production, controlled rearing conditions, reduced allergen concerns, and the valorization of an otherwise discarded biomass. Overall, this approach strengthens the economic viability of BSF biorefineries while supporting the European Green Deal and the transition toward a fully circular and bio-based cosmetic industry.

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Preparation of Polyvinyl Alcohol (PVA) Magnetic Composites with Nickel-Zinc Ferrite Nanoparticles for Magnetic Hyperthermia Applications

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Magnetic hyperthermia is a technique based on the physical response of certain materials—typically magnetic nanoparticles—that dissipate energy as heat when exposed to an alternating magnetic field [1]. Its fundamental principle—generating localized, controlled heat at the nanoscale—has been explored in applications such as oncology, tissue engineering, drug delivery, and environmental remediation. This versatility has driven interest in designing magnetic materials that allow for the optimization of the technique and greater control over material functionality [2].

In this study, nickel-zinc ferrite nanoparticles were synthesized via the chemical co-precipitation method, yielding an average particle size of 18.53 ± 5 nm as determined by TEM. These particles were dispersed in a 2 wt% polyvinyl alcohol (PVA) matrix. The matrix was allowed to dry to immobilize and support the particles and restrict the contribution of Brownian relaxation (physical rotation of the particle), thereby allowing for the predominant observation of Néel relaxation (internal rotation of the magnetic moment) [3].

The powdered material was structurally and morphologically characterized using XRD, TEM, and Raman spectroscopy. The material within the polymer matrix was characterized using impedance spectroscopy and the Rowland ring method. The results obtained thus far aim to contribute to the design of materials with controllable magnetic properties for applications in magnetic hyperthermia.

The authors gratefully acknowledge the support of the DGAPA-PAPIIT IN113624 project for financial support.

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DEVELOPMENT OF COPPER OXIDE-POLY(2-HYDROXYETHYL METHACRYLATE-CO-N-VINYLCAPROLACTAM) NANOCOMPOSITES FOR USING AS SMART DRUG DELIVERY PLATFORM

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Hybrid nanocarriers based on metal oxide nanoparticles (NPs), such as copper oxide (CuO), combined with stimuli-responsive polymers have demonstrated great potential for taregted and controlled release of anticancer drugs [1]. Among these polymers, poly(*N*-vinylcaprolactam) (PNVCL) have shown thermoresponsive behavior around physiological temperature [2], while delivery systems based on poly-2-hydroxyethylmethacrylate (PHEMA) have exhibited pH-dependent release [3,4].

In this work, CuO NPs, previously functionalized with an organosilane agent, were coated with poly(HEMA-co-NVCL) *via* surface initiated free radical polymerization. Nanocomposites with different percentage of copolymer grafting were obtained by varying comonomer feed ratio and reaction time. These nanohybrids were characterized by Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and transmission electron microscopy (TEM); their hydrodynamic size (Dh) and behavior in colloidal dispersion was determined by dynamic light scattering (DLS) and Z-potential (ζ). Furthermore, they demonstrated the ability to load 5-Flouroruracil (5-FU) and doxorrubicin (DOX).

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Hybrid CdTe/PEDOT: PSS solar cells combining polymers with different conductivities

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Hybrid CdTe/PEDOT:PSS solar cells were processed by incorporating the PEDOT:PSS polymer between the CdTe absorbing semiconductor and the Cu-Mo back contacts. The PEDOT: PSS was prepared combined in different proportions with two distinct providers and with different conductivities. Providers Hereaus (H) and Aldrich (A) report conductivities for their different PEDOT: PSS of 0.002 and >200 S/cm, respectively; property that can be influence of the photovoltaic parameters of hybrid CdTe/PEDOT: PSS solar cells. The different proportions of the two distinct polymers were (H:A) in a 1 ml of volume were: 1:0, 3:1, 2:1, 1:1, 1:2, 1:3 and 0:1. The average thickness of the PEDOT: PSS was measured by profilometry and it was of 40 nm ± 3 nm, and the optical transmittance remained without change and close to 80% in the range from 300 nm to 1000 nm; while the resistivity varying 10^2 to 10^{-3} Ω-cm, for these different proportions. Hybrid SnO_2:F/ZnO+CdS/CdTe/PEDOT: PSS (H:A) solar cell was obtained and characterized by I vs V and EQE. The best solar cells was obtained when the proportion was 1:3, with the following photovoltaic parameters: V_{oc} =0.742 V, J_{sc}= 21.3 mA/cm^2, FF= 0.45 and η=8.8%. These results were correlated by measuring spectral quantum efficiency with a maximum intensity close to 65%.

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Effect of PEIE concentration on the photovoltaic response of CdTe-based solar cells

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To prepare ethoxylated polyethyleneimine (PEIE) polymer for organic solar cells, PEIE is dissolved in methanol [1]. In this work, we study the variation in PEIE concentration with respect to methanol concentration in the ranges of 1:50, 1:100, and 1:150 (PEIE:methanol) and its effect on the photovoltaic response of inorganic CdTe solar cells. The PEIE was prepared with the following proportional amounts for: 1:50, 24 mg of PEIE and 1200 mg of methanol; for 1:100, 12 mg of PEIE and 1200 mg of methanol; and for 1:150, 10 mg of PEIE and 1500 mg of methanol. The PEIE was deposited using a spin coating equipment with the following experimental parameters: a volume of 200 µl, rotation speed of 5000 rpm for 30 seconds of deposition time. The average thickness of the PEIE as measured by profilometry was 26 nm ± 3 nm, and the optical transmittance was close to 99% in the range from 300 nm to 1000 nm.
This result were used in the following SnO_2:F/PEIE/CdS/CdTe/Cu-Mo solar cell structure, and these solar cells were compared with a reference solar cell without PEIE.
The best solar cells was obtained when the polymer concentration was 1:150, with the following photovoltaic parameters: V_{oc} =0.673 V, J_{sc}= 19.1 mA/cm^2, FF= 0.47 and η=7.0% and for the reference solar cell, V_{oc} =0.687 V, J_{sc}= 17.9 mA/cm^2, FF= 0.43 and η=6.1%. These results were correlated by measuring spectral quantum efficiency with a maximum intensity of 55%.

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Abstract preparation

PVA-Ciprofloxacin Nanofibers: Study about the Impact of Superficial Modification

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This study focuses on the effect of covalently bonding an antibiotic to the surperficie of a polyvinyl alcohol (PVA) nanofiber system; the goal is to observe how this affects both the composite's microstructure and the antimicrobial response of the drug used. To this end, ciprofloxacin (a potent antibiotic of broad-spectrum from quinolone family) [1] was extracted from a commercial tablet and covalently bonded to PVA nanofibers via an ester linkage formed with the antibiotic's carboxylic acid group. The material was characterized using spectroscopic analysis (FTIR-ATR), field-emission scanning electron microscopy (FESEM), thermal analysis (TGA and DSC), and X-ray photoelectron spectroscopy (XPS); mechanical, biocompatibility, and microbiological tests will also be conducted. Additionally [2],[3], the ciprofloxacin will be modified before to covalent bonding using bis(2-chloroethyl) ether as a linking molecule connecting the antibiotic's piperazine ring to the PVA to determine how this modification alters properties such as antimicrobial activity. These materials show potential for use as wound dressings for cutaneous wounds, creating an antiseptic environment at the application site.

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Photophysical dynamics of two aminophosphonates and two aminophosphinates and its TD-DFT interpretation: a sound photodissociation

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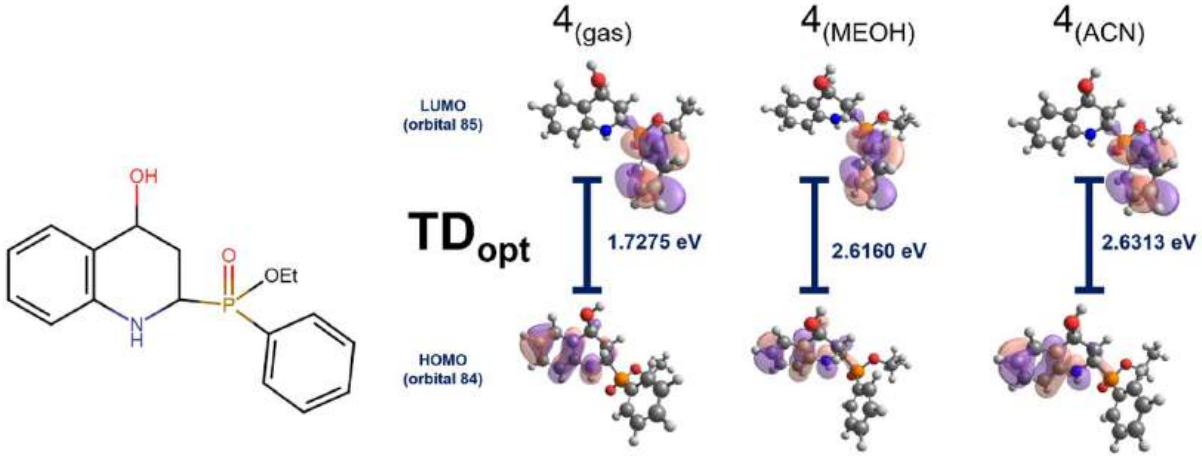
Despite the structural difference between phosphinate and phosphonate groups, as both are bioisosters of natural aminoacids, they feature different numbers of phosphorous-carbon and phosphorous-oxygen bonds. Under visible irradiation, the aromatic system is responsible of absorption for both systems, nevertheless the received energy is diverted into a fluorescent state with preference for the photodissociation in only one of the studied species using methanol dissolution, according to the TD-DFT calculations perfomed under PCM methodology. Additionally, synthesis experimental data in synthesis assures the spectroscopy and computational data of the phosphinate as a leaving group under visible irradiation.



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POCOP Pincer Compounds. A Modular Approach for the Desing and Synthesis of Metallopharmaceuticals in the Battle Against Cancer

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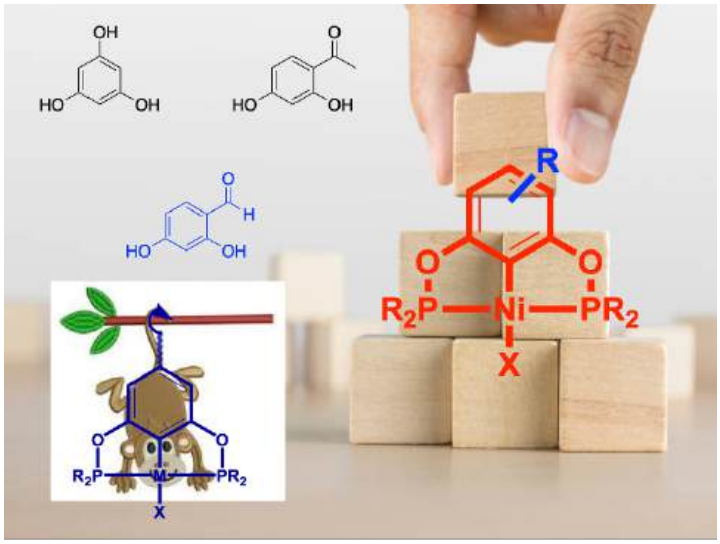
In this talk we will present recent results on the use of POCOP pincer compounds as privileged motif for the modular design and synthesis of organometallic species and the exploration of their cytotoxic activities in the battle against Cancer.



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DEVELOPMENT OF AN OXYGEN-RELEASING ALGINATE-BASED BIOMATERIAL FOR β-CELL ENCAPSULATION

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Introduction: Oxygen deprivation remains a principal limitation to the success of pancreatic β-cell encapsulation strategies for the treatment of type 1 diabetes. The development of biomaterials capable of providing localised oxygen supplementation may improve cell survival and preserve cellular functionality following encapsulation. **Objective:** To evaluate the potential of calcium peroxide-containing alginate hydrogels as oxygen-generating matrices for pancreatic β-cell support. **Methods:** Composite hydrogels based on alginate, graphene oxide, calcium peroxide, and poly-L-lysine were developed and characterised. Oxygen generation, mechanical stability, rheological behaviour, and biological performance were assessed using pancreatic β-cell cultures encapsulated within the constructs. **Results:** The incorporation of calcium peroxide enabled sustained oxygen release for several days, generating a more favourable microenvironment for encapsulated cells. Material characterisation demonstrated that oxygen-generating formulations preserved the structural integrity and viscoelastic properties required for cell encapsulation. Biological analyses revealed improved cellular compatibility and metabolic activity in oxygen-releasing hydrogels compared with non-supplemented formulations. Notably, the formulation containing 0.25% calcium peroxide showed the best overall performance, combining adequate oxygen delivery with favourable material properties and cellular responses. **Conclusion:** Oxygen-generating hydrogels represent a promising strategy to overcome hypoxic stress in encapsulated pancreatic β-cells. The optimised formulation developed in this study provides sustained oxygen availability while maintaining suitable physicochemical characteristics, highlighting its potential application in future cell-based therapies for type 1 diabetes.

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Oxygen-Releasing Collagen Hydrogel Enhances the Viability and Functionality of Pancreatic β Cells for Diabetes Cell Therapy

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Introduction: Type 1 diabetes is characterised by the progressive loss of insulin-producing β cells, creating a need for innovative strategies that improve cell survival and functionality after transplantation. Biomaterial-based encapsulation systems have emerged as promising platforms; however, limited oxygen availability within the cellular microenvironment remains a major challenge affecting graft performance. To address this issue, an oxygen-generating, collagen-based hydrogel was engineered by combining a type I collagen matrix with a poly(ethylene glycol) diacrylate (PEGDA) interpenetrating network and incorporating vascular endothelial growth factor (VEGF) and calcium peroxide (CPO) as an oxygen source. **Methods:** Physicochemical characterisation demonstrated successful integration of all hydrogel components while preserving the structural features of native collagen. The incorporation of CPO enhanced the scaffold's mechanical properties and enabled sustained oxygen delivery for approximately 8 days. The biological performance of the system was assessed by exposing pancreatic β cells to different CPO concentrations. Among the tested formulations, the hydrogel containing 0.25% CPO exhibited the most favourable response, maintaining high cell viability and promoting cellular growth throughout the evaluation period. **Results:** Furthermore, β cells cultured within this oxygen-releasing platform showed improved metabolic activity, evidenced by increased cellular respiration and enhanced insulin secretion compared with non-oxygenated controls. These findings indicate that controlled oxygen supplementation within a collagen-based hydrogel can effectively mitigate hypoxic stress and support β-cell function. **Conclusion:** Overall, the VEGF-functionalized collagen/PEGDA hydrogel containing 0.25% calcium peroxide represents a promising biomaterial platform for pancreatic β-cell encapsulation and may contribute to the development of advanced cell-based therapies for diabetes management.

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SYNTHESIS AND CHARACTERIZATION OF AN MAA–EGDMA MOLECULARLY IMPRINTED POLYMER AS A BIORECEPTOR PLATFORM: A DESIGN-OF-EXPERIMENTS STRATEGY

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Molecularly imprinted polymers (MIPs) provide versatile nanostructured platforms for synthetic bioreceptors. In this study, poly(methacrylic acid-co-ethylene glycol dimethacrylate) (PMAA–EGDMA) coatings were synthesized on polystyrene nanoparticles by $FeCl_2$/ascorbic-acid-initiated redox polymerization at room temperature. Scanning electron microscopy revealed formulation-dependent morphological changes, with the most favorable conditions preserving a continuous fibrillar network. Electrical impedance spectroscopy (20 Hz–10 MHz) was used to compare MIP and non-imprinted polymer (NIP) samples (n = 9 per group). At 20 Hz, the NIP exhibited a higher impedance magnitude than the MIP (|Z| = 13.56 vs. 12.76 kΩ). At 10 MHz, however, the NIP showed a lower impedance magnitude (3.47 vs. 3.63 kΩ) and a more negative phase angle (θ = −71.3° vs. −66.5°), indicating stronger high-frequency capacitive behavior. At 100 kHz, the NIP also showed higher conductance (6.51×10^{-4} vs. 2.52×10^{-4} S), while the Nyquist plots displayed a larger negative imaginary component (−Im(Z) = 4622 vs. 4008 Ω). Collectively, these differences show that molecular imprinting modifies the frequency-dependent electrical response of the polymer, with the MIP exhibiting a comparatively more resistive behavior under the evaluated conditions. Based on these findings, a design-of-experiments (DoE) strategy is proposed to optimize the monomer-to-crosslinker ratio and template concentration and to relate morphological and electrical responses to cavity accessibility, binding capacity, and selectivity in bioreceptor applications.

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Lighting Up Amphiphilic Janus Dendrimers: From Molecular Design and Self-Assembly to Cellular Imaging

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Amphiphilic Janus dendrimers (AJDs) are a class of dendrimers composed of hydrophilic and hydrophobic segments. These macromolecules can undergo self-assembly in aqueous media to form various nanostructures, including micelles, tubules, cubosomes, ribbons and vesicles, depending on their molecular structure and hydrophilic–hydrophobic balance [1]. Dendrimer-derived vesicles, known as dendrimersomes, are of particular interest due to their resemblance to biological membranes and their potential applications in drug delivery and nanomedicine. In this context, incorporating molecules with aggregation-induced emission (AIE), such as tetraphenylethylene (TPE), can provide inherently fluorescent nanoassemblies without the aggregation-caused quenching associated with conventional fluorophores.

In this talk, we discuss the synthesis of two families of TPE-functionalized AJDs and their self-assembly in aqueous media. We first present AJDs with varying generation numbers and discuss the effects of their molecular structure and self-assembly conditions on the morphology and photophysical properties of the resulting nanoassemblies [2]. By controlling these parameters, fluorescent dendrimersomes with tunable diameters of approximately 60–200 nm and quantum yields of 5.7–17.4% were obtained. We will then discuss the use of activated alkyne–hydroxyl click chemistry as a mild and metal-free method for the synthesis of AJDs containing π-extended TPE units [3]. These macromolecules exhibited AIE in aqueous media and self-assembled into fluorescent micelles or dendrimersomes depending on their generation number. The extended conjugation of the TPE units enabled their visualization using conventional confocal microscopy. Finally, the biocompatibility and efficient cellular uptake of these nanoassemblies will be presented, highlighting their potential as fluorescent materials for cellular imaging and future theranostic applications.

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Rational Design of Well-Defined Ether-Free Aromatic Polymers for Energy Conversion, Storage, and Catalytic Applications

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The development of chemically robust polymeric materials is crucial for next-generation energy technologies, including fuel cells, water electrolyzers, redox flow batteries, and suoercapacitors. Among these, anion exchange membranes (AEMs) have attracted considerable attention as promising low-cost alternatives for electrochemical energy conversion and storage systems. However, achieving high ionic conductivity while maintaining chemical and mechanical stability under alkaline conditions remains a major challenge. Conventional aromatic AEMs based on poly(arylene ether ketone)s and poly(arylene ether sulfone)s offer attractive performance, yet their ether-containing backbones are vulnerable to degradation in harsh alkaline environments.

Herein, we report a versatile and scalable synthetic platform for the preparation of wholly aromatic, ether-bond-free polymers via superacid-catalyzed polyhydroxyalkylation of carbonyl compounds with activated and non-activated aromatic monomers. This metal-free Friedel–Crafts-type methodology enables the synthesis of well-defined, linear, soluble, and high-molecular-weight polymers under mild conditions, providing structurally diverse backbones with superior chemical robustness and high thermal stability.

Through postpolymerization functionalization, different ionic and catalytic functionalities were introduced, including quaternary ammonium, imidazolium, pyridinium, and redox-active moieties, allowing precise modulation of ion exchange capacity (IEC), water uptake (WU), ionic conductivity, and electrochemical behavior. The resulting materials were processed into membranes and thin films and characterized by FT-IR, ^{1}H and ^{13}C NMR, DSC, TGA, intrinsic viscosity, morphology, and mechanical analysis.

Structure–property relationships demonstrated that the modularity of this synthetic strategy enables the design of multifunctional polymers suitable not only for AEMs in hydrogen production and fuel cells, but also as ion-conducting binders and separators for electrochemical capacitors, as well as catalytic platforms for heterogeneous and electrocatalytic processes. These results establish polyhydroxyalkylation as a powerful and versatile tool for the development of advanced aromatic polymeric materials for energy storage, energy conversion, and catalysis.

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FUNCTIONALIZATION OF PVA NANOFIBERS WITH ELASTIN AS A BIOMEDICAL SCAFFOLD FOR TETRACYCLINE RELEASE

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The extracellular matrix (ECM) is a dynamic and highly organized environment that regulates essential processes such as cell adhesion, proliferation, and differentiation. In particular, the anisotropic arrangement of its fibrillar components plays a fundamental role in cell orientation and the distribution of biochemical signals [1]. Therefore, the development of biomaterials capable of reproducing the structural and functional characteristics of the ECM represents one of the main strategies in tissue engineering and controlled drug delivery systems [2].

In this context, nanofibers obtained by electrospinning stand out as versatile platforms due to their high surface-to-volume ratio, high porosity, and ability to mimic the fibrillar architecture of native tissues [3]. This project explores the influence of the orientation of polyvinyl alcohol (PVA) nanofibers functionalized with tetracycline (TTC), incorporated via physical adsorption and post-fabrication covalent functionalization strategies. The effect of fibrillar alignment on drug-release kinetics is evaluated to develop systems that reduce the initial burst-type release and promote a more sustained, controlled release over time [4]. The structural characterization of the resulting biomaterials is performed using field-emission scanning electron microscopy (FE-SEM). They are also characterized using FTIR spectroscopy and TGA/DSC thermal analysis to confirm drug incorporation and evaluate their physicochemical stability. This is complemented by in vitro release studies to establish the relationship among the orientation of the nanofibers, the mechanism of tetracycline incorporation, and the release profile of the developed system.

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DEVELOPMENT OF A THREE-DIMENSIONAL SYSTEM BASED ON BACTERIAL NANOCELLULOSE FOR *IN VITRO* EVALUATION OF COLON CANCER DRUGS.

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In 2026, the International Agency for Research on Cancer reported that Annual cancer cases are projected to rise to nearly 35 million by 2050, moreover, colorectal cancer (CRC) is the third most common cancer type worldwide [1]. Cancer drug evaluation involves in vitro assays, animal studies, and clinical trials. Traditionally, two-dimensional (2D) cell cultures have been used as the first stage for drug development. Neverletheless, they do not reproduce cell–cell interaction [2],[3],[4]. Bacterial nanocellulose (BNC) is a sustainable material with significant potential for biomedical applications because of its high purity, biocompatibility, and mechanical properties, however, it lacks of a 3D macrostructure to create CRC 3D model. Accordingly, we decide to explore the development of a three-dimensional system based on BNC for *in vitro* evaluation of colon cancer drugs.

The material was produced using paraffin molds, and after purification, a 3D structure was revealed. BNC 3D was characterized into safetty using ISO 10993 and then its performance using CRC cell lines was evaluated and compared against Matrigel® and under perfusion using a CRC drug (5-Flourouracil). BNC 3D showed no evidence of cytotoxicity, genotoxicity, or mutagenicity. Based on its performance NCB 3D showed a functional equivalence between matrices, with viability exceeding 85% without statistically significant differences and a higher proportion of cells in the G2/M phase compared to the 2D culture or Matrigel®. Evaluation of 5-fluorouracil in 2D, static 3D, and perfused 3D culture revealed increasing drug resistance with system complexity: the IC_{50}(3D)/IC_{50}(2D) ratio reached up to 20 in SW620 (metastatic cell line) at 48 h, moreover under continuous perfusion, no model achieved 50% inhibition at the reference IC_{50} established in 2D. These results position BNC 3D as a dynamic, reproducible, and biocompatible platform, with a greater capacity to reveal differences in drug resistance between cell lines than conventional systems.

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Maleic Acid-Grafted Poly(vinylpyrrolidone) Hydrogels Synthesized by Gamma Radiation for pH-Responsive Drug Delivery

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Hydrogels are highly relevant materials due to their unique properties, such as softness, flexibility, and biocompatibility [1]. Structurally, hydrogels are three-dimensional molecular networks linked by covalent or non-covalent bonds [2]. Due to the presence of polar groups in their structure, such as SO_3H, OH, NH_2, COOH, and $CONH_2$, they can absorb considerable amounts of water or biological fluids, maintaining network integrity while remaining in a swollen state [3]. Therefore, they are widely studied in various fields, including drug delivery, tissue engineering, and regenerative medicine [2,3]. In this research, PVP hydrogels net(PVP) were synthesized and subsequently grafted with maleic acid net(PVP)-g-MA by gamma radiation. These hydrogels were then loaded with naringin and antimicrobial agents for controlled release, aiming to develop pH-responsive materials that prevent infections and promote faster tissue regeneration. Under the selected experimental conditions, an MA grafting degree of approximately 18% was achieved. The hydrogels were characterized by attenuated total reflectance Fourier-transform infrared spectroscopy, differential scanning calorimetry, thermogravimetric analysis, and swelling studies. The results confirmed the successful incorporation of MA into the hydrogel network and demonstrated that the grafting process imparted pH-responsive behavior through the ionization of the carboxylic acid groups, with two critical pH values identified at 4.4 and 6.0. Loading and release studies using naringin and benzalkonium chloride showed that the grafted hydrogels exhibited an enhanced loading capacity and sustained release profiles governed by the hydrogel network and the interactions between the loaded compounds and the carboxylic groups of MA. Furthermore, hydrogels loaded with antimicrobial agents effectively inhibited the growth of *Escherichia coli* and *Staphylococcus aureus*.

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Two-stage radiation-induced grafting of N,N-dimethylacrylamide and N-vinylcaprolactam onto polypropylene for ciprofloxacin loading and release

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Polypropylene films were functionalized through a two-step radiation-induced grafting process using N,N-dimethylacrylamide and N-vinylcaprolactam to obtain drug-loading materials with improved hydrophilic and thermoresponsive properties. Grafting was performed by the oxidative pre-irradiation method using gamma radiation. DMAAm grafting reached values close to 36%, whereas NVCL grafting onto previously modified PP-g-DMAAm films achieved a maximum of approximately 19%. FTIR-ATR analysis confirmed the successful incorporation of both monomers onto the PP surface. Swelling studies showed a marked increase in water uptake with increasing grafting percentage, reaching approximately 16% for PP-g-DMAAm and 26% for (PP-g-DMAAm)-g-NVCL. Thermal analysis revealed that the NVCL-containing material exhibited an apparent temperature-dependent response with a transition at approximately 45 °C, which may be associated with a change in the hydration state of the grafted NVCL. Ciprofloxacin loading and release studies demonstrated that PP-g-DMAAm films were capable of incorporating and releasing the antibiotic. Antimicrobial assays against Escherichia coli and Staphylococcus aureus confirmed that ciprofloxacin-loaded PP-g-DMAAm films retained antibacterial activity. These findings demonstrate the potential of radiation-grafted PP films as antibiotic-releasing materials and provide preliminary evidence that incorporating NVCL can impart thermoresponsive behavior.

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DESIGN AND SYNTHESIS OF ENGINEERING POLYMERS FOR SELECTIVE GAS SEPARATION: STRUCTURE-PROPERTY RELATIONSHIPS.

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Keywords: ROMP, polynorbornendicarboximides, gas separation.

Polymeric membranes have become established as a promising alternative for selective gas separation due to their lower energy consumption, operational simplicity, and ease of scale-up compared to conventional technologies such as absorption or cryogenic distillation. These advantages have driven their application in processes such as CO_2 capture, hydrogen purification, and natural gas sweetening. However, the development of new materials remains a challenge due to the intrinsic trade-off between permeability and selectivity [1–3].

In this work, the synthesis of two membranes based on polynorbornen dicarboximides is reported: poly-[*N*-2-fluoro-4-(trifluoromethyl)phenyl-*exo*-norbornen-5,6-dicarboximide](poly-PhNDID) and poly-[N-4-(triphenylmethyl)phenyl-exo-norbornen-5,6-dicarboximide] (poly-PhNDIE), synthesized via ROMP using the second-generation Grubbs catalyst. These materials differ in the nature of the pendant group, allowing the study of the relationship between chemical structure and gas transport properties.

Dense membranes were prepared by solving casting and characterized thermally, mechanically, and structurally. Both materials exhibited excellent thermal stability (Td > 400 °C) and glass transition temperatures above 200 °C, reflecting the rigidity of the polymer chains. Additionally, tensile tests showed elastic modulus values above 1600 MPa and ultimate tensile strength above 35 MPa. X-ray diffraction analysis confirmed the formation of amorphous polymers.

Gas transport properties (He, H_2, O_2, N_2, CH_4, and CO_2) were evaluated at 35 °C and 2 atm using a constant-volume method. The poly-PhNDID membrane showed significantly higher permeabilities for all gases (P (CO_2) = 55.36 Barrers) compared with the poly-PhNDIE membrane (P (CO_2) = 4.38 Barrers), attributed to the increased free volume generated by the presence of

bulky fluorinated groups. In contrast, poly-PhNDIE exhibited higher selectivity, associated with improved packing of the polymer matrix.

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Chitosan-Alginate Nanoparticles for Insulin Release

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Insulin therapy remains one of the mainstays of diabetes mellitus treatment; However, the limitations associated with conventional administration routes have driven the development of alternative delivery systems capable of protecting insulin and promoting its controlled release [1-3]. The objective of this study was to design, synthesize, and characterize chitosan–alginate nanoparticles as a system for the encapsulation of recombinant human insulin and to evaluate their potential for pH-responsive release at pH 4.5 and 7.4.

The nanoparticles were synthesized by ionic crosslinking, using sodium tripolyphosphate (TPP) as the crosslinking agent. Physicochemical characterization was performed by UV–Vis spectroscopy, attenuated total reflectance Fourier-transform infrared spectroscopy (FTIR–ATR), dynamic light scattering (DLS), zeta potential analysis, and fluorescence spectroscopy.

The resulting nanoparticles exhibited an encapsulation efficiency of 30±2.6% and a zeta potential of +41±1.7 mV at pH 4.0. The positive surface potential is consistent with the presence of protonated amino groups in chitosan and suggests adequate electrostatic stabilization of the dispersion under acidic conditions. The spectroscopic and physicochemical results were consistent with the incorporation of recombinant human insulin into the chitosan–alginate matrix. The response of the system to pH changes between 4.5 and 7.4 highlights the relevance of electrostatic interactions between the matrix components and the protein, which may influence insulin retention and release.

In conclusion, chitosan–alginate nanoparticles represent a promising platform for the encapsulation of recombinant human insulin. Their physicochemical properties and pH-dependent behavior support their further investigation as a controlled-release system.

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Addressing Poor Drug Solubility: From Supramolecular complexes to Nanostructured Delivery Systems

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Poor aqueous solubility remains a major challenge in the development and formulation of pharmaceutical compounds, limiting drug dissolution, bioavailability, and therapeutic performance. In some applications, however, the goal is not necessarily to increase bioavailability, but to provide an appropriate delivery system that maintains the drug in a soluble or dispersed state, preventing precipitation in the circulation and enabling it to reach the intended target site. Since poor solubility may arise from different molecular and solid-state properties, no single formulation approach can provide a universal solution. Instead, different strategies can be selected according to the physicochemical characteristics of the drug and the intended pharmaceutical application.

In this talk, three complementary approaches to improve the solubility and delivery of poorly water-soluble drugs are discussed, ranging from molecular-level interactions to nanostructured delivery systems. First, cyclodextrins are presented as supramolecular hosts capable of increasing apparent drug solubility through inclusion complexation and additional non-covalent interactions [1]. Second, liposomes, lipid-based vesicles capable of encapsulating poorly soluble drugs, are presented as delivery systems that can maintain drugs in a dispersed state, facilitating their transport to biological targets while preventing precipitation in the systemic circulation [2]. Third, electrospun membranes, solid matrices composed of micro- or nanoscale fibers, can be designed to disperse poorly soluble compounds for local or systemic delivery, taking advantage of their high surface area and rapid hydration to favor drug dissolution and release [3]. Their comparison highlights the importance of selecting formulation strategies according to drug properties and the intended application rather than considering solubility enhancement as a one-size-fits-all problem. At the Instituto de Investigaciones en Materiales, we explore molecular complexation, lipid-based encapsulation, and polymeric nanostructured matrices to address poor aqueous drug solubility, while investigating their fundamental mechanisms toward the development of innovative and feasible therapeutic solutions.

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Acrylamide hydrogels functionalized with aldehyde groups obtained by gamma-radiation-induced grafting

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The incorporation of aldehyde functional groups into polymeric materials has gained increasing importance due to their high reactivity and ability to form dynamic covalent bonds [1,2]. In this study, a new aldehyde-functionalized hydrogel was developed by grafting a vanillin-derived monomer onto an acrylamide hydrogel via gamma-radiation-induced free-radical copolymerization. The monomer was synthesized by reacting vanillin with acryloyl chloride and was characterized using FTIR-ATR and mass spectrometry. The resulting grafted hydrogels were systematically characterized via FTIR-ATR, SEM, TGA, DSC, and swelling measurements to evaluate their structural, thermal, and physicochemical properties. The results confirmed the successful incorporation of aldehyde groups arranged in a comb-like architecture within the copolymer network. The hydrogels exhibited a porous morphology with an average pore size of 3.079 ± 0.682 µm and a high swelling capacity of approximately 2000% in aqueous and simulated physiological media. Furthermore, the chemical reactivity of the aldehyde groups was confirmed through covalent bonding with phenylalanine via imine formation, highlighting the potential of these materials for further functionalization. These findings provide valuable insights for designing functional polymer networks with tunable physicochemical properties and reactive sites for advanced material applications.

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PMPC-b-PDMAEMA block copolymers for gene delivery: "DNA complexation induced by template polymerization"

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Nowadays, gene delivery for therapeutic purposes is considered one of the most promising strategies to treat both genetic and acquired diseases, such as cancer. However, nucleic acid delivery faces numerous extra- and intracellular barriers, limiting transfection efficiency. Consequently, the development of safe and efficient gene delivery vectors remains a major challenge for the targeted delivery of genes to specific tissues or cells. Therefore, the investigations on non-viral gene vectors with the ability to overcome physiological barriers are increasing and efficiently delivering nucleic acids into target cells. Amphiphilic block copolymers have attracted considerable interest due to their tunable chemical composition and their ability to self-assemble into nanostructures capable of protecting and transporting genetic material [1]. In this context, the aim of this work is to develop amphiphilic block copolymers in aqueous medium for applications in nanomedicine and nucleic acid encapsulation and release. To this end, a water-soluble segment of poly(2-Methacryloyloxyethyl Phosphoryl Choline) (PMPC) is synthesized via RAFT polymerization and combined with a cationic segment of 2-dimethylaminoethyl methacrylate (DMAEMA), capable of condensing and delivering nucleic acids into cells using a novel "template" approach based on DNA complexation [2], working with DNA concentrations up to 40 mg/mL. The resulting nanoparticles were characterized using DLS (D_H ~ 150 nm), ζ-potential (+18 mV), TEM and SAXS (fractal like structures).

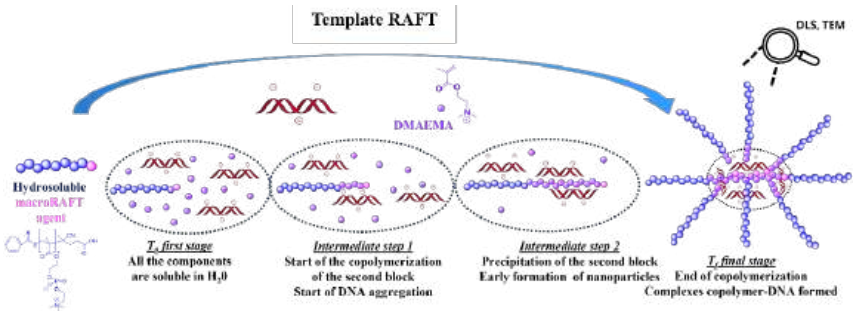

Figure 1: Schematic representation of the DNA template RAFT steps.

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ITACONIC ACID-FUNCTIONALIZED POROUS POLYMER MONOLITHS FOR CONTINUOUS-FLOW CATALYSIS: PERMEABILITY AND CATALYTIC PERFORMANCE

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Functionalized porous polymers are promising materials due to their potential in diverse applications, including their use as support media for catalysts. In this work, polystyrene-divinylbenzene-itaconic acid (PS-DVB-AI) monoliths were synthesized with dimensions of 2 cm in height and 0.8 cm in diameter by Pickering emulsion polymerization. This synthetic route enables the formation of a bicontinuous morphology, which is markedly different from the cellular porous structures typically obtained by polyHIPE polymerization. In this system, itaconic acid not only introduced carboxylic acid functional groups into the polymer matrix, whose presence was confirmed by Fourier-transform infrared spectroscopy (FTIR) through the C=O stretching vibration at 1720–1706 cm^{-1}, but also contributed to the mechanical rigidity of the monoliths. The effect of formulation variables, specifically the dispersed monomer-phase fraction in the Pickering emulsion, the crosslinking agent (DVB), porogen (hexadecane), and silica nanoparticles, on the final permeability of the monoliths was investigated. For this purpose, the pressure drop at different volumetric flow rates was measured, and the corresponding permeability factors were calculated. The results showed that the monomer-phase fraction and crosslinking agent had the greatest influence on the final permeability of the columns, with higher DVB contents and lower monomer-phase fractions resulting in greater pressure drops. Based on these results, the monolith exhibiting the lowest pressure drop was selected for evaluation as a catalytic support. This material was impregnated with the precursor salt $Pt(NH_3)_4Cl_2 \cdot xH_2O$, followed by Pt reduction to obtain the catalytically active phase. The catalytic performance of the material was evaluated through the aqueous-phase reduction of 4-nitrophenol to 4-aminophenol in a continuous-flow system, using different volumetric flow rates ranging from 0.5 to 4 mL/min. The highest conversion (98%) was achieved at a flow rate of 0.5 mL/min, which provided the longest residence time and consequently, the highest catalytic conversion (98%). Finally, the reactive column was evaluated under continuous operation to assess its stability and catalytic performance over time. The column could be operated continuously for 12 hours without a significant decrease in conversion, maintaining a conversion of 98% after 1 hour of operation and 96% after12 hours.

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From Plastic Waste to Advanced Materials: A Strategy for the Generation of Carbonaceous Structures.

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Carbon fiber is a high-performance material that plays an important role in the automotive industry due to its mechanical strength and light weight—essential attributes for reducing vehicle weight. Currently, more than 90% of the fibers available on the market are derived from polyacrylonitrile (PAN), a precursor that significantly increases production costs and limits its widespread use [1]. At the same time, the accumulation of polyolefin plastics, such as polypropylene (PP), poses a serious environmental challenge due to their lack of biodegradability. The purpose of this study is to develop an alternative and sustainable method for producing carbon fibers using polypropylene waste as a precursor, through a pyrolysis process.

To ensure the structural stability of the material and prevent the polypropylene from melting prematurely, the polypropylene fibers undergo a thermal and oxidative stabilization process to induce effective cross-linking of the polymer chains. Following this, the material is subjected to a pyrolysis process in an inert atmosphere [2]. Initial physicochemical characterization via X-ray diffraction confirmed that the precursor had a monoclinic phase, while thermogravimetric analysis helped determine the mass loss rates. The resulting fibers are expected to exhibit competitive properties for practical applications, thereby promoting recycling and the circular economy.

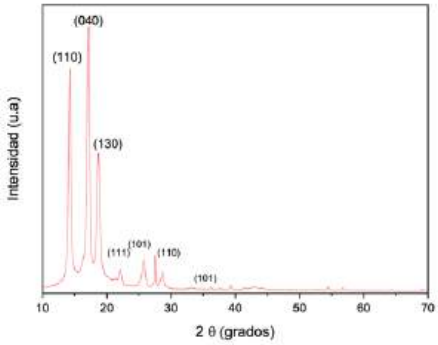

Figure 1. DRX PP

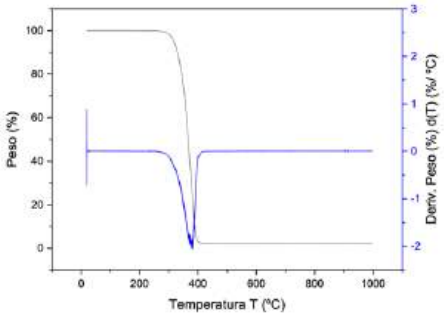

Figure 1. TGA PP

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File Naming

Valorization of lignin for composites and biomedical applications

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Lignin, the most abundant aromatic bioplymer in Earth, is a structural component of plant cell walls. Processing of wood into pulp and paper results in enormous lignin waste, that is burned to recover energy. However, lignin is a valuable material that can be used in a variety of applications that range from composites with polyolefins to nanomaterials for biomedical uses. In this contribution we show results from kraft lignin surface modification with non-equilibrium plasmas to improve the compatibility with polypropylene at significant lignin contents. On the other hand, lignin was isolated from tequila agave bagasse and corncob, two relevant agro-industrial residues in Mexico, through organosolv and alkaline processes to be used as a building block for the development of lignin-based biomaterials. FTIR and NMR results showed that both lignins are composed of syringyl and guaiacyl units, while XPS revealed a higher contribution of surface hydroxyl groups in agave lignin and carbonyl functionalities in corncob lignin. Both lignins exhibited bacteriostatic activity against *S. aureus* (>96%). Lignin nanoparticles were synthesized, as described in [1], using formaldehyde as crosslinking agent at 18 and 27 wt. %. Sunscreen was prepared by mixing with a commercial body cream and ZnO nanoparticles at 5 wt. % and varying amounts of lignin NPs (5-15 wt. %), yielding SPF from 4-13; lignin NPs showed absorption in the UVB and UBC regions [2]. Corncob or tequila agave bagasse lignin hydrogels were synthesized using polyethylene glycol diglycidyl ether (PEGDGE) or 1,4-butanediol diglycidyl ether (BDDE) as crosslinkers. Corncob lignin hydrogels showed cell viability above 70%, higher swelling capacities, reaching up to 400% in PBS and 800% in water, while both hydrogels showed a predominantly elastic behavior (G′ > G″), characteristic of crosslinked hydrogel networks. These findings demonstrate the relevance of lignin source and chemistry in tailoring hydrogel properties and support the valorization of agro-industrial lignins for the development of sustainable biomaterials.

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POLYMERIC EUTECTOGELS FOR CONTROLLED CURCUMIN DELIVERY AND TISSUE REGENERATION

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Enhancing the bioavailability and stability of curcumin (CUR) are essential to optimize its therapeutic potential in cancer treatment. It has been addressed by complexing it with β-CD [1] and by using deep eutectic solvents (DES) [2]. The incorporation of DES into polymer matrices enables the formation of supramolecular eutectogels (SE), which are biocompatible and adhesive materials suitable for the controlled release of CUR [3]. In this work, we developed a controlled-release CUR delivery system based on a polyvinyl alcohol/chitosan/hyaluronic acid (PVA/CTS/HA) matrix in the form of a SE. β-CD-based DES were used to form β-CD/CUR inclusion complexes and to promote the SE formation, thereby improving the long-term stability of CUR. The PVA/CTS/HA mixture was prepared at a 2:1:1 v/v ratio. CUR was solubilized in the following DES: choline chloride/glycerol (ChCl/Gly, 1:1 molar ratio), β-CD/formic acid (β-CD/FA, 1:90 molar ratio) and 2-hydroxypropyl-β-CD/formic acid (HPβ-CD/FA, 1:90 molar ratio). FT-IR analysis confirmed the supramolecular interactions between the polymers and the formation of inclusion complexes between the CUR and the DES, as shown in Figure 1. Furthermore, *in vitro* release studies demonstrated the controlled release of CUR from the SE prepared with β-CD /AF. In addition, the PVA/CTS/HA mixture exhibited antibacterial activity against *S. aureus*, which may contribute to preventing infection and promoting the wound-healing process. Overall, the resulting ES materials are bifunctional, providing controlled CUR delivery while simultaneously promoting tissue regeneration and wound healing.

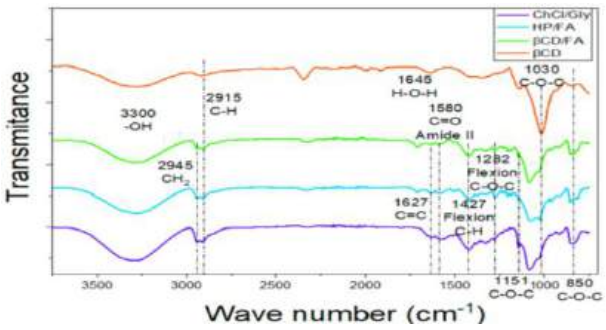

Figure 1. *FT-IR spectrum of ES and β-CD powder.*

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SYNTHESIS, CHARACTERIZATION, AND HEAVY METAL ADSORPTION PROPERTIES OF POLYNORBORNENE DICARBOXIMIDES

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Over the past several decades, the development of ring-opening metathesis polymerization (ROMP) has led to a wide range of commercial, scientific, and technological applications. This versatile polymerization technique has enabled the synthesis of novel materials with well-defined chemical structures that are difficult to obtain using conventional polymerization methods. In this context, norbornene-based monomers have attracted considerable attention because the functional polymers derived from them exhibit favorable thermomechanical and chemical properties, making them promising candidates for applications as adsorbents for the removal of heavy metal ions, including Pb^{2+}, Cd^{2+}, and Ni^{2+}, from aqueous media. Based on these considerations, this work reports the synthesis and ring-opening metathesis polymerization (ROMP) of novel norbornene imide monomers using a second-generation Grubbs catalyst. Dense polymer membranes were prepared by casting approximately 8 wt% polymer solutions in DMF at 45 °C, followed by slow solvent evaporation. The chemical structure and thermal properties of the synthesized monomers and polymers were characterized by FT-IR spectroscopy, NMR spectroscopy, thermomechanical analysis (TMA), and thermogravimetric analysis (TGA), among other techniques. The heavy metal ion uptake of the polymer membranes was quantified by atomic absorption spectrometry.

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Abstract preparation

THREE-DIMENSIONAL FUNCTIONALIZED HYDROGEL NETWORK FOR BETA PANCREATIC CELLS ENCAPSULATION

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Type I collagen is one of the main components of extracellular matrix in many tissues, including pancreas, and it is widely used as biocompatible material [1]; however, it has low mechanical stability. To improve this characteristic, it has been purposed to form an interpenetrated network (IPN) with poly (ethylene glycol) diacrylate (PEGDA) [2]. IPNs are promising in tissue engineering and three-dimensional cell culture, despite of their reduced cell viability. This study explores the functionalization of collagen-PEGDA IPNs with vascular endothelial growth factor (VEGF) at concentrations 1, 3 and 5 ng/mL to enhance biocompatibility and support pancreatic β cell survival. Physicochemical characterization showed a biomaterial where the different components added were integrated including PEGDA and VEGF. Moreover, the mechanical properties show stability of a tunable hydrogel with adequate stiffness and degradation rate to stand several days of incubation. Biocompatibility assays showed that the functionalized hydrogel platformed supported cell viability and promoted cell proliferation better than the non-functionalized hydrogel. These results suggest that collagen/PEGDA IPN hydrogel at VEGF concentration of 3 ng/mL and 5 ng/mL could provide a better environment for the functional capacity of pancreatic β cells for further studies.

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Abstract preparation

SYNTHESIS AND CHARACTERIZATION OF ZIF-8 AND ZIF-67 FOR GAS SEPARATION

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Metal-organic frameworks (MOFs) are a class of crystalline inorganic-organic hybrid materials composed of a metal ion or clusters of metal ions linked by di-, tri-, or tetradentate organic ligands, primarily through coordination bonds [1]. In particular, MOFs are ideal materials for gas storage and separation due to their large surface areas, tunable pore sizes, and controllable surface properties [2]. To address the performance and stability challenges associated with polymeric membranes, alternative materials have been developed for formulating new separation systems. These materials include components known as metal-organic frameworks (MOFs), which are used both to form membranes and as fillers within a polymer matrix to create mixed-matrix membranes. Processing MOF-based membranes often generates high-flux pathways that compromise membrane selectivity during gas separation; consequently, the most common application involves incorporating MOF nanoparticles as fillers in a polymer matrix. However, mixed-matrix membranes present interfacial challenges between the organic and inorganic phases [3].In this work the synthesis and characterization of ZIF-8 and ZIF-67, was carried out through methanol and solvothermal methods. Synthesis conditions for obtaining these compounds were determined, and parameters such as reaction time and the metal source-to-ligand molar ratio were varied to achieve a better reaction yield. The characterization techniques used Fourier Transform infrared spectroscopy (FT-IR), UV-Vis and X-Ray Diffraction.

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IMPRINTED POLYMERS EMBEDDING IRON(III) COMPLEXES FOR DYE POLLUTANT REMOVAL: TOWARD GREEN AND EFFICIENT WASTEWATER REMEDIATION

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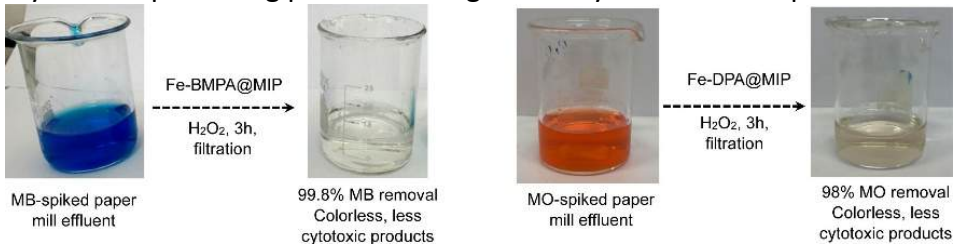
Dye pollutants from textile and related industries are highly recalcitrant, posing significant environmental and health risks. In this study, we evaluate a family of Fe(III) complexes and their corresponding molecularly imprinted polymers (MIPs) as efficient, green catalysts for the oxidative degradation of the dyes methyl orange (MO), methylene blue (MB), and malachite green (MG). Solution studies revealed that the nature of the ligand influences the relative contributions of radical-mediated and high-valent Fe(V)=O oxidation pathways, enabling tunable reactivity. The most active complexes were used as templates to generate water-compatible MIPs that combine adsorption with Fenton-like degradation. The best-performing MIPs were those containing the bis(2-pyridylmethyl)amine or dipicolinic acid complexes (Fe-BMPA@MIP and Fe-DPA@MIP). Both achieved 73–99% dye decolorization within 3 h while minimizing iron leaching, and converted the dyes into lower molecular weight products with reduced cytotoxicity. A test conducted in dye-spiked paper-mill effluent further confirmed the high decolorization efficiency of the polymers under realistic conditions (see the figure). These results highlight Fe(III)-complex-imprinted polymers as promising platforms for greener dye wastewater pre-treatment.



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Influence of Formulation Pathway on PEI/DNA Polyplexes Properties and Gene Delivery

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Polymer-based vectors are widely used for nucleic acid delivery, including mRNA vaccines and gene therapy. They condense nucleic acids (NAs) into nanoparticles, protect them from nuclease degradation and facilitate their intracellular delivery. Polycations form polyplexes with NAs through electrostatic interactions. While traditional approaches mainly focus on polymer chemistry and charge ratio (R = $[N^+]/[P^-]$), increasing evidence indicates that formulation kinetics and mixing conditions also play an important role in polyplex compaction, structure and stability. Polyethylenimine (PEI) is widely studied for gene delivery due to its high charge density and ability to form stable nanoparticles [1]. Here, branched PEI (25 kg/mol) was used as a model polycation to investigate how the order, volume and kinetics of PEI and DNA addition affect polyplexes properties and biological activity, evaluated through green fluorescent protein (GFP) expression in HEK293T cells. Two formulation strategies were compared: rapid addition with vortex mixing and slow, progressive addition under gentle stirring. Polyplexes were prepared at a charge ratio of 10 to maintain a polycation excess and promote efficient transfection. Their size and surface charge were characterized with Dynamic Light Scattering (DLS) and ζ-potential measurements, and GFP expression was assessed in HEK293T cells after 24 h. Rapid mixing produced smaller particles (~42 nm), whereas slow addition resulted in larger particles (~110 nm). Interestingly, it was found that the biological activity also depended on the formulation pathway and the relative volumes of PEI and DNA: formulations prepared using equal volumes of both components showed significantly lower GFP expression than those prepared with a larger plasmid volume relative to PEI. These results highlight the importance of formulation conditions in determining polyplex properties and biological activity, even at a fixed charge ratio.

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CORRELATION BETWEEN RHEOLOGICAL BEHAVIOR, SURFACE TENSION, AND ELECTROSPINNABILITY IN PECTIN–PEO SYSTEMS WITH CURCUMIN AND PIPERINE

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Pectin is a renewable and biocompatible polysaccharide with potential for the development of electrospun materials [1]; however, its limited chain entanglement can hinder the formation of continuous fibers. Blending pectin with polyethylene oxide (PEO) improves its processability, although the electrospinning behavior of these systems remains dependent on the physicochemical properties of the precursor solutions [2]. Furthermore, the incorporation of bioactive compounds may modify these properties and consequently affect fiber formation. This work aims to characterize the rheological behavior and surface tension of pectin-PEO solutions with and without curcumin and piperine, and to establish their correlation with electrospinnability and the morphology of the resulting structures. Formulations containing different pectin and bioactive compound concentrations will be evaluated under controlled preparation and electrospinning conditions. Rheological and surface properties of the precursor solutions will be characterized and related to their behavior during electrospinning, including jet stability and the formation of continuous or defective structures. The morphology of the electrospun materials will subsequently be analyzed to assess changes in fiber formation associated with solution composition. This study seeks to establish correlations between the physicochemical properties of pectin-PEO precursor solutions and their electrospinning behavior, providing insight into the effect of polymer concentration and curcumin/piperine incorporation on the formation of electrospun fibrous materials.

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Session 2. Computational and Hybrid Materials

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Abstract

Influence of the orientation of organic cations on carrier recombination and its correlation to photovoltaic efficiency in MAPbI3 hybrid perovskite

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Organic–inorganic hybrid perovskites exhibit remarkable optoelectronic properties, including long carrier lifetimes and strong light absorption. In $MAPbI_3$, the methylammonium (MA) cation is dynamically disordered at high temperature, and its reorientation is coupled to local distortions of the PbI6 framework. Here, fixed MA orientations are treated as representative local snapshots of pseudo-cubic $MAPbI_3$ to examine their effect on electronic, optical, and radiative-limit properties. Using HSE+SOC first-principles calculations, we analyze six MA-orientation snapshots and compute band gaps, absorption spectra, radiative recombination coefficients, carrier lifetimes, and SLME-derived photovoltaic metrics. The band gap varies from 1.34 to 1.51 eV, giving radiative lifetimes of 47-73 ns and SLME efficiencies from 28.1 to 31.1%. Diagonal-like configurations provide the most favorable absorption-voltage balance.

Computer Simulations of Contaminant Capture on Solid Surfaces and in Water Using Surfactant Molecules

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Using molecular dynamics simulations, we investigated the potential of surfactant molecules as an efficient alternative for contaminant remediation. First, the ability of surfactant micelles to capture CO_2 in water was investigated using different micellar structures prepared with sodium dodecyl sulfate (SDS) and biosurfactants. Simulations were performed at different gas concentrations and temperatures, and the results showed that biosurfactant micelles enhanced CO_2 retention. Furthermore, adsorption isotherms were calculated and fitted to the Langmuir model. The results demonstrated that micelle structure plays a key role in CO_2 retention. Molecular dynamics simulations were also employed to investigate the desorption of hydrocarbons from solid surfaces as an efficient remediation strategy. Two surfactants, a synthetic surfactant, sodium dodecyl sulfate (SDS), and the biosurfactant surfactin, were combined with hexanol and simulated over a range of surfactant concentrations. Density profiles were calculated to characterize the interactions between the surfactants, hydrocarbons, and solid surfaces. The results showed that surfactin promoted hydrocarbon desorption more effectively than SDS from cellulose surfaces, indicating a greater ability to disrupt hydrocarbon–surface interactions. Overall, these findings the simulations demonstrated that surfactants significantly enhance the removal of various contaminants, highlighting their potential as alternative agents in decontamination processes.

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Polymat Contributions

Bridging Physics, Chemistry, and Materials Science Through Molecular Simulations

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Molecular simulations have become an essential tool for understanding and predicting the behavior of materials at the atomic and molecular scales. These computational approaches provide a bridge between fundamental physics, chemistry, and materials science, enabling researchers to investigate systems that are often difficult or expensive to study experimentally. Central to molecular simulations are *force fields*, mathematical models that describe how atoms and molecules interact.

This seminar will present a general overview of the development of modern force fields and their role in the simulation of complex molecular systems. The talk is intended for a broad scientific audience and will introduce the basic concepts behind molecular simulations.

Particular attention will be given to the methodology used to construct and validate force fields[1]. The seminar will discuss how computational methods combine experimental data, statistical mechanics, and electronic structure calculations to produce transferable and predictive molecular models. Special attention will also be given to recent developments in electrolyte modeling used in divices to storage energy [2], advanced intermolecular potentials, and the implementation of computational methodologies for molecular simulations in complex fluids and hybrid materials [3].

The overall goal is to provide a broad perspective on how molecular simulations contribute to modern materials research and how they are becoming increasingly important in chemistry, physics, biology, and engineering.

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2. Molecular dynamics simulations for liquid electrolytes of propylene carbonate with LiTFSI, $LiPF_6$, and $LiBF_4$ salts. J. Molec. Liq, **2023**, 390, Part A, 122983. E. Núñez-Rojas, I. González, G. Guzmán-González, J. Alejandre.
3. Efficient search of molecular interaction parameters for polar liquids. Molec. Phys, **2024,** 122, (19-20). J. Pozos-García, E. Núñez-Rojas, J. L. Quiroz-Fabián, A.Pérez-Espinosa, J. Alejandre

COMPETITIVE ADSORPTION OF HEAVY METALS IN SYNTHETIC AND BIOLOGICAL MICELLES: A MOLECULAR DYNAMICS APPROACH

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Heavy metal contamination presents a significant environmental challenge, requiring efficient and sustainable remediation strategies. In this study, we use molecular dynamics (MD) simulations to evaluate and compare the performance of synthetic sodium dodecyl sulfate (SDS) and biological Rha-C10-C10 rhamnolipid micelles in removing divalent heavy metals, specifically Cd^{2+}, Co^{2+}, Ni^{2+}, and Zn^{2+}. Computational models were constructed, and the Radial distribution functions, charge density profiles, and intrinsic electric fields were computed to elucidate the binding mechanisms at the micelle-water interface. Our results demonstrate distinct competitive binding affinities, notably highlighting the specific anomalous radial distribution peak of nickel, as well as the strong coordination behavior of cobalt ions with the micellar polar heads. These atomistic insights provide a fundamental understanding of how biosurfactants can serve as eco-friendly alternatives to traditional synthetic surfactants for heavy metal remediation in wastewater treatment.

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Oxidation-Driven Electronic and Optical Modulation in Silicon Nanowires

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Silicon nanowires (SiNWs) are promising materials for nanoelectronic, photonic, and sensing applications due to their tunable physicochemical properties.[1,2] Under ambient conditions, silicon surfaces spontaneously oxidize, leading to the formation of Si/SiO_x interfaces that strongly affect their electronic and optical behavior.[3] In this work, first-principles density functional theory calculations were employed to investigate the evolution of the electronic and optical properties of progressively oxidized ⟨100⟩ silicon nanowires. The results reveal a continuous reduction of the direct band gap from 2.00 to 1.17 eV as oxidation proceeds. Band structure and projected density-of-states analyses show that the valence-band edge remains dominated by Si states from the crystalline core, whereas the conduction-band minimum is strongly influenced by Si–O environments at the interface. Consequently, band-gap narrowing is mainly driven by a downward shift of interfacial conduction-band states. Oxidation also induces a progressive redshift of the optical absorption onset and a decrease in the intensity of the dielectric response. Charge-density analyses demonstrate that the electronic redistribution associated with oxidation is highly localized at the Si/SiO_x interface. These findings identify the interface as the key region controlling the electronic structure and optical response of oxidized silicon nanowires, providing insights for the design of silicon-based optoelectronic and sensing devices.

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EXPERIMENTAL AND COMPUTATIONAL STUDY OF COMPOSITE ALUMINUM FOAMS REINFORCED WITH CERAMIC PARTICLES

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Metallic foams constitute a significant advancement in materials science, as they combine low density with high mechanical strength. Their porous architecture, inspired by natural materials such as bone or coral, provides efficient and sustainable engineering solutions. These materials are suitable for both structural and functional applications due to their ability to significantly reduce weight while maintaining excellent energy absorption capacity, which is particularly advantageous for safety-related uses. In addition, metallic foams exhibit recyclability, corrosion resistance, and stability at elevated temperatures. The addition of ceramic particles into aluminum foam matrices improves compressive strength, energy absorption, and structural stability, particularly when a uniform distribution is achieved [1]. Nevertheless, the mechanical properties highly depends on the wettability of the reinforcement, generally low for molten metals. That is why the possible formation of matrix-reinforcement interfacial regions is critical It is reported that Finite Element Modeling (FEM) accurately predicts the mechanical response of these materials, but the appropriate selection of the Representative Volume Element (RVE) and the interfacial bonding strength is of critical importance [2]. This work combines experiments and simulations to study how interfacial bonding influences the Young's modulus of aluminum foams reinforced with Al_2O_3 and $Al(OH)_3$.

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Polymat Contributions

Bridging Physics, Chemistry, and Materials Science Through Molecular Simulations

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Molecular simulations have become an essential tool for understanding and predicting the behavior of materials at the atomic and molecular scales. These computational approaches provide a bridge between fundamental physics, chemistry, and materials science, enabling researchers to investigate systems that are often difficult or expensive to study experimentally. Central to molecular simulations are *force fields*, mathematical models that describe how atoms and molecules interact.

This seminar will present a general overview of the development of modern force fields and their role in the simulation of complex molecular systems. The talk is intended for a broad scientific audience and will introduce the basic concepts behind molecular simulations.

Particular attention will be given to the methodology used to construct and validate force fields[1]. The seminar will discuss how computational methods combine experimental data, statistical mechanics, and electronic structure calculations to produce transferable and predictive molecular models. Special attention will also be given to recent developments in electrolyte modeling used in divices to storage energy [2], advanced intermolecular potentials, and the implementation of computational methodologies for molecular simulations in complex fluids and hybrid materials [3].

The overall goal is to provide a broad perspective on how molecular simulations contribute to modern materials research and how they are becoming increasingly important in chemistry, physics, biology, and engineering.

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Abstract preparation

EXPERIMENTS AND THEORY ON THE RHEOLOGY OF COMPLEX SYSTEMS.

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In this conference we present experimental results on the Rheology of complex materials and their theoretical description by a new approach named Connectivity Field Theory. To understand the flow of complex materials requieres model systems with fine experiments and constitutive models that may predict, optimistically, the basic behavior of these systems, with clear simplicity to be implemented numerically with demanding computational codes.

Giant micellar systems are model compounds which may provide experimental data to motivate their prediction by suitable analytical and computational models contained in the new theories. Under flow, the relevant relaxation mechanisms combine the breakage-reformation process of the micelles and the simulateneus polymer-like reptation mechanisms. These processes are examined under different flow situations like stress relaxation, inception of shear, large amplitude oscillatory flow, hysteresis, creep and considering yield-stress materials. The dynamics of these systems are similar to those observed in metals and ceramics, thereby allowing a generalisation to hybrid-materials description.

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First-Principles Evaluation of MoS_2/Phosphorene Heterostructures for Photocatalytic Water Splitting

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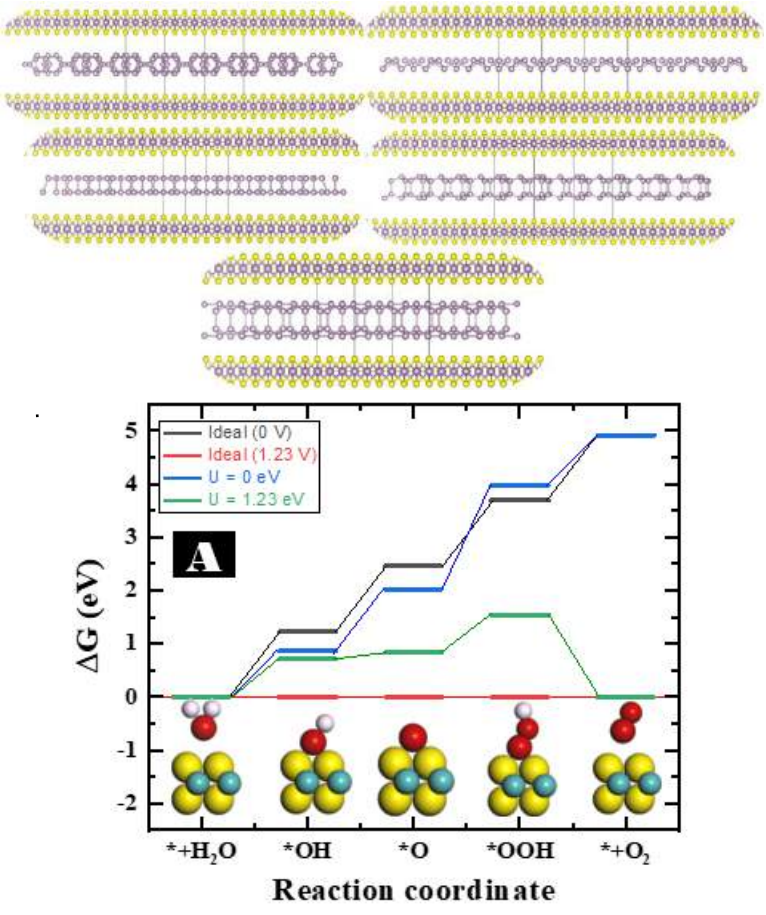
ABSTRACT

In this study, we explore the potential of novel two-dimensional materials for energy conversion by investigating five distinct configurations of phosphorene (PX = Hex-Hex, v-Mono-$(P2)_{trans}$, p-Hex-$(P2)_{trans}$, v-Hex-$(P2)_{cis}$, and Mono-(P4)). By evaluating fundamental properties such as their band gaps, work functions, and band edge positions, we reveal how coupling these phosphorene configurations with MoS_2 creates highly versatile heterostructures MoS_2@PX. First-principles calculations demonstrate that these new structures maintain excellent dynamic and thermal stability, even at elevated temperatures, while exhibiting strong optical absorbance across the visible light spectrum. Employing the HSE06 approximation, we confirm that these heterostructures are robust semiconductors with widely tunable band gaps ranging from 1.69 to 3.42 eV, heavily dependent on the basic units assembled within the network. Most importantly, the conduction band (E_{CB}) and valence band (E_{VB}) edges of specific allotropes align favorably with the redox potentials of H_2/H^+ and O_2/H_2O. This optimal band alignment, paired with their visible-light absorption capabilities, positions these tunable phosphorene/MoS_2 heterostructures as highly promising candidate materials for visible-light-driven photocatalytic water splitting.



ZnO Nanowires for optical biodetection of multidrug-resistant E. coli.

Rafael A. Salinas[1], Shirlley Elizabeth Martinez Tolibia[1], Citlaly Gutiérrez Rodelo[2], Laura Jeanette García Barrera[3], Rogelio Zapata Arenas[4], Juliana Gutiérrez Rodelo[5], Andrés Navarrete[2], Ateet Dutt[6], Guillermo Santana[6], Carlos Ramos Vilchis[1]

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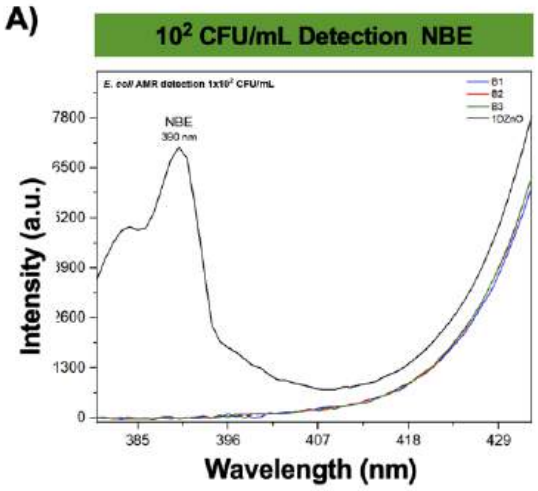
Medical treatment innovations coupled with nanotechnology have resulted in great advancements for bioimaging, drug-delivery, gene therapy, personalized medicine, pathogen biosensing, among others. This synergy has been successful due to the advantages provided by nanomaterials such as small size and morphologies, large surface-to-volume ratio, and ease of surface modification to increase biocompatibility, which have promoted an enhanced interaction with cells at intracellular and extracellular levels. Antimicrobial resistance (AMR) is a global phenomenon that has strongly impacted on the health of humans, animals, and ecosystems, which can end up in a huge pandemic outbreak in the upcoming future. In this regard, taking advantage of the luminescent properties of 1DZnO as biosensing nanoplatforms for pathogen detection, we performed experiments for detection of AMR E. coli (ampicillin and erythromycin resistant), providing increased functionalities of nanowires. First, the biofunctionalization of NWs by hydroxylation and subsequent silanization using APTMS was carried out, as reported previously. Then, polyclonal antibodies against E. coli were used to promote the immobilization of these bioreceptors over functionalized 1DZnO, placed in contact with antibody solutions (50 µg/mL). Biofunctionalized substrates were used for fast detection of multidrug-resistant E. coli, from bacterial dilutions adjusted at 10^4 CFU/mL and 10^2 CFU/mL, establishing short contact times (10 s ±2) between substrates and bacterial samples. 1DZnO substrates were washed three times in 500 µL sterile water, and PL spectra observed the presence of attached bacteria. Photoluminescence detection was performed by triplicate, and statistical analyses evaluated the obtained spectra from each concentration to characterize the specificity of the optical response and the differences between both concentrations detected of AMR E. coli. After contact with bacterial cells, it is observed an interference with the optical response, derived from the biological components from bacterial membranes such as phospholipids, porins, peptidoglycans, etc. involved in the quenching of the PL signal, a behavior that is observed both at $1x10^4$ and $1x10^2$ CFU/mL. This profile is consistent in all tested 1DZnO nanoplatforms and their replicates (B1, B2, and B3), corroborating that the peak area from NBE presents a prominent decrease, also observed in DLE, that are inversely proportional to the detected concentration



Keywords: E. coli, Biodetection, AMR bacteria

Addressing Poor Drug Solubility: From Supramolecular complexes to Nanostructured Delivery Systems

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Poor aqueous solubility remains a major challenge in the development and formulation of pharmaceutical compounds, limiting drug dissolution, bioavailability, and therapeutic performance. In some applications, however, the goal is not necessarily to increase bioavailability, but to provide an appropriate delivery system that maintains the drug in a soluble or dispersed state, preventing precipitation in the circulation and enabling it to reach the intended target site. Since poor solubility may arise from different molecular and solid-state properties, no single formulation approach can provide a universal solution. Instead, different strategies can be selected according to the physicochemical characteristics of the drug and the intended pharmaceutical application.

In this talk, three complementary approaches to improve the solubility and delivery of poorly water-soluble drugs are discussed, ranging from molecular-level interactions to nanostructured delivery systems. First, cyclodextrins are presented as supramolecular hosts capable of increasing apparent drug solubility through inclusion complexation and additional non-covalent interactions [1]. Second, liposomes, lipid-based vesicles capable of encapsulating poorly soluble drugs, are presented as delivery systems that can maintain drugs in a dispersed state, facilitating their transport to biological targets while preventing precipitation in the systemic circulation [2]. Third, electrospun membranes, solid matrices composed of micro- or nanoscale fibers, can be designed to disperse poorly soluble compounds for local or systemic delivery, taking advantage of their high surface area and rapid hydration to favor drug dissolution and release [3]. Their comparison highlights the importance of selecting formulation strategies according to drug properties and the intended application rather than considering solubility enhancement as a one-size-fits-all problem. At the Instituto de Investigaciones en Materiales, we explore molecular complexation, lipid-based encapsulation, and polymeric nanostructured matrices to address poor aqueous drug solubility, while investigating their fundamental mechanisms toward the development of innovative and feasible therapeutic solutions.

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DATA-DRIVEN IDENTIFICATION OF MoO_2 AND MoO_3 PHASE DISTRIBUTIONS IN MOLYBDENUM OXIDE–SILICON SEMICONDUCTOR INTERFACES USING SEM-EDS ANALYSIS

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The integration of molybdenum oxide (MoO_x) thin films on silicon substrates represents a promising strategy for the development of high-efficiency semiconductor devices. However, the spatial identification of the different oxide phases present at the interface, particularly MoO_2 and MoO_3, remains a challenge due to the inherent limitations of conventional characterization techniques and the complexity of the data obtained using Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS). In this work, a data science-based algorithm was developed to process SEM-EDS elemental maps and facilitate the identification and visualization of regions associated with different molybdenum oxidation states. The algorithm analyzes the stoichiometric relationships between molybdenum and oxygen, allowing the distinction of MoO_2 and MoO_3-enriched zones and the graphical representation of their distribution within the sample. The results obtained show a significant improvement in the interpretation of the chemical heterogeneity of the semiconductor-oxide interface, providing relevant information on deposition, oxidation, and heat treatment processes. This methodology contributes to a more precise characterization of MoO_x-based semiconductor materials, facilitating the correlation between phase distribution and the functional properties of the device. Furthermore, it demonstrates the potential of data science tools to complement and strengthen the analysis of advanced materials using SEM-EDS techniques, in accordance with recent advances in artificial intelligence applied to the characterization of semiconductor materials [1, 2, 3, 4].

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Parametric optimisation of triply periodic minimal surface reinforced tubular structures.

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Triply periodic minimal surfaces (TPMS) can be used to design advanced cellular materials with applications in thermal systems, fluid transport and catalysis, and as structural materials. This work focuses on developing a design methodology for TPMS-based cellular solids, as illustrated by the optimisation of a cylinder reinforced by a skeletal Schwarz diamond structure with a thickness gradient in the radial direction. Optimisation uses the response surface methodology, with the following parameters: structural thickness (t), δt, which represents the increase in thickness, and n, which defines the sharpness of the structural gradient. Dependent variables are are the thickness of the outer wall and the relative density of the structure.

To provide a restriction on the design, surfaces of constant relative density were calculated in the 3-dimensional design space and restricted by the minimal wall and structure thickness. For the minimal permittable density, ten points were selected on the corresponding iso-surface to model the apparent modulus and compressive strength of the cylinders. Triangle mesh 3D models were then generated for each these points, followed by manual repair of mesh defects, triangulation of quadrangular elements and tetragonal mesh conversion.

Finite-element simulations imposed a 2% downward displacement upon the upper face of the cylinder. Z-axis reaction force values were then extracted from the simulation results, from which the apparent elastic modulus and maximal stress are calculated. Interpolation between the ten simulation points then allows to calculate the optimal thickness and gradient parameters. Overall, this methodology offers a scalable and reproducible foundation for engineering tailored TPMS-based cellular materials.

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Abstract preparation

Computational Study of Ibuprofen Adsorption on Carbonaceous Materials via DFT Calculations: Analysis of Molecular Descriptors

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Ibuprofen ($C_{13}H_{18}O_2$), a nonsteroidal anti-inflammatory drug, persists in aquatic effluents at ng/L–µg/L levels despite conventional wastewater treatment [1]. Using DFT (R^2SCAN-3c/ORCA 6.0.1) with GFN2-xTB pre-optimization and DOCKER conformational search, benzene adsorption was evaluated as a molecular probe on PAHs, fullerenes (C60–C74), SWCNTs, and graphene oxide/reduced graphene oxide (GO/rGO) [2]. Adsorption energies (Eads), benchmarked against literature CCSD(T)/CBS values, followed the trend PAHs > SWCNTs > fullerenes: affinity increased with π-domain size in PAHs, while surface curvature weakened interactions in fullerenes and nanotubes. rGO with a moderate C/O ratio showed the best balance between π–π stacking and oxygenated anchoring sites, favoring hydrogen-bonding with ibuprofen. These results highlight π-domain extension and surface topology as key drivers of adsorption, positioning partially reduced graphene oxide as a rationally designed adsorbent for water treatment [3].

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Abstract preparation

Suitable formation of Zn[X=S or Se](en)$_{0.5}$ hybrid films on Zn foils for photocatalytic applications in the environmental and energy fields

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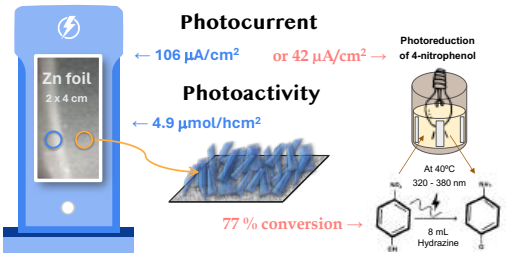
Nanocomposite semiconducting thin film materials have achieved a revolutionary impact in various fields including healthcare, environmental and energy applications [1]. Thin films are categorized as two-dimensional (2D) materials as their thickness is within the nanometer range [2]. A new family of hybrid nanocomposites based on ZnS or ZnSe and amine ligands (such as ethylenediamine) has been explored for their interesting physicochemical properties due to their unique lamellar-sheet nanostructures [3]. The inorganic layers spaced by diamine ligands promote efficient conduction pathways for electron-hole pairs to improve the transport properties when it is grown on zinc foil. This study focuses on suitable formation of ZnS(en)$_{0.5}$ and ZnSe(en)$_{0.5}$ hybrid on zinc metal foil using solvothermal method in a ternary mixture of solvent. The nanocomposite hybrid films show photocatalytic activity for H_2 production [4] or photoassisted 4-nitrophenol reduction reaction [5]. The physicochemical parameters and the photocatalytic properties are correlated with photoelectrochemical behavior.



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Abstract

DECIPHERING THE ANTIBACTERIAL AND CYTOTOXIC EFFECTS OF 1DZnO NANOPLATFORMS

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From the last decades, ZnO-based nanomaterials have exhibit great potential, wide versatility, and diversified physico-chemical properties to be incorporated in different applications involving biological systems. Such properties are size, morphology, nanostructural defects, synthesis methods, isoelectric point, and surface-to-volume ratio which can determine their functionality across various systems. For instance, morphologies of ZnO nanomaterials, such as nanoparticles (NPs), nanorods (NRs), tetrapods, and nanowires (NWs) seem to play an interesting role in cell-nanomaterial interaction, which require targeted characterizations.
In this work, we performed independent experiments to test the antibacterial activity of ZnO NWs against Gram-negative bacteria, and biocompatibility after interaction with mammalian cells.
The experimental setup of the antibacterial behavior was evaluated through the agar diffusion method, where ZnO NWs were placed up-side at the center of agar plates.
According to our results, moderate antibacterial activity of raw ZnO NWs was confirmed by the presence of inhibition halos against ampr-E.coli, providing updated behavior on the effects of nanowires interaction with bacterial membranes. Contrastingly, biocompatible interactions with HEK-293 cells were observed, demonstrating that ZnO NWs did not affect the substrate surrounding cells, thereby preserving morphological characteristics and viability rates, suggesting a stable bioavailability under direct contact with HEK-293. Novel nanotechnological approaches are needed to explore not only the ability to inhibit bacterial growth but also to ensure that their development is suitable for further *in vivo* assays, and effective in the long term [1].
These results provide reference for further fabrication of eco-friendly biosensing devices based on ZnO NWs, which could represent a sustainable innovation for high-throughput detection.

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S. E. M. T. (CVU 703157) thankfully acknowledges the CONAHCyT/SECIHTI postdoctoral fellowship and the grant provided by L´Oréal- UNESCO-AMC for women in science. Thankfully, R. A. S. (CVU 703153) acknowledges the CONAHCyT/SECIHTI postdoctoral fellowship. C. G. R. thankfully acknowledges the PAPIIT project IA209426. A. D. thanks the Project PAPIIT-DGAPA-UNAM IN100125.

EXPERIMENTAL AND COMPUTATIONAL STUDY OF COMPOSITE ALUMINUM FOAMS REINFORCED WITH CERAMIC PARTICLES

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Metallic foams constitute a significant advancement in materials science, as they combine low density with high mechanical strength. Their porous architecture, inspired by natural materials such as bone or coral, provides efficient and sustainable engineering solutions. These materials are suitable for both structural and functional applications due to their ability to significantly reduce weight while maintaining excellent energy absorption capacity, which is particularly advantageous for safety-related uses. In addition, metallic foams exhibit recyclability, corrosion resistance, and stability at elevated temperatures. The addition of ceramic particles into aluminum foam matrices improves compressive strength, energy absorption, and structural stability, particularly when a uniform distribution is achieved [1]. Nevertheless, the mechanical properties highly depends on the wettability of the reinforcement, generally low for molten metals. That is why the possible formation of matrix-reinforcement interfacial regions is critical It is reported that Finite Element Modeling (FEM) accurately predicts the mechanical response of these materials, but the appropriate selection of the Representative Volume Element (RVE) and the interfacial bonding strength is of critical importance [2]. This work combines experiments and simulations to study how interfacial bonding influences the Young's modulus of aluminum foams reinforced with Al_2O_3 and $Al(OH)_3$.

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Optical bands in bi-chiral photonic structures with twist defects

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A theoretical analysis is conducted on the optical spectra of solid structurally bi-chiral media with local point-group symmetry $\bar{4}2m$ exhibiting the Pockles effect and containing twist defects. The system is composed of two adjacent layers of helical structure with constant pitch, each having a helix of opposite handedness and a twist defect located at the center of the layer. Right- and left-circularly polarized electromagnetic waves are obliquely incident on the system. Its spectral properties are studied for different values of the medium parameters, twist defect angles and applied electric field intensities along the helical axis of the medium. The transmittances and reflectances are computed using the transfer matrix method within the piecewise uniform approximation. In these systems, universal optical defect modes that are insensitive to the polarization state are observed, thereby enabling the design and fabrication of electrically controlled universal narrowband optical filters.

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Laura O. Palomares acknowledges financial support from the Sistema Nacional de Investigadores e investigadoras (SNII) of CONAHCYT, Mexico.

Supramolecular Cation Engineering of Blue-Excitable $[Cu_4I_6]^{2-}$ Cluster Phosphors

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Lead-free copper(I) halides are attractive luminescent materials because they combine high photoluminescence quantum yields (PLQYs) with versatile processing. However, many all-inorganic low-dimensional copper halides require high-energy UV excitation, limiting their use as phosphor converters driven by commercial blue LEDs [1]. Discrete zero-dimensional $A_2[Cu_4I_6]$ cluster phosphors provide an alternative route toward visible-light excitation while retaining broadband, efficient emission [2]. Their stabilization, however, typically relies on bulky organic cations, whereas smaller ammonium species favor extended Cu-I frameworks. Expanding the available cation chemistry therefore remains a key synthetic challenge.

Here, we introduce a supramolecular strategy in which 18-crown-6 (18C6) acts as a host for NH_4^+, methylammonium (MA^+), and phenethylammonium (PEA^+), effectively converting small ammonium species into larger supramolecular cations capable of stabilizing copper iodide cluster architectures [3]. This host-guest approach enables systematic modification of the organic environment surrounding the emissive $[Cu_4I_6]^{2-}$ unit without requiring a new covalent cation scaffold for each composition. Single-crystal X-ray diffraction and Hirshfeld surface analysis show that the topology of H···I, H···Cu, and intercluster I···I contacts controls cluster distortion, water incorporation, and lattice relaxation. These structural changes directly modulate exciton-phonon coupling and emission bandwidth, while density functional theory calculations confirm strong localization of the band-edge states within the copper iodide clusters. Across the series, increasing cation steric bulk and hydrophobicity progressively suppresses structural disorder and water incorporation; PEA(18C6) combines approximately 80% PLQY with improved thermal and moisture stability and efficient blue-driven white-light emission. These results establish supramolecular cation engineering as a modular route to expand the chemical space of blue-excitable copper(I) cluster phosphors and tune their structural, photophysical, and environmental properties.

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Broadband White Emission LED from $C_4N_2H_{14}PbBr_4$-Based 1D Perovskite

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One-dimensional (1D) organic–inorganic hybrid perovskites have attracted significant interest due to their strong quantum confinement and broadband emission driven by self-trapped excitons (STEs). [1,2] Here, we report the first 1D white-light-emitting perovskite LED (PeLED) based on $C_4N_2H_{14}PbBr_4$ (Figure 1). The device exhibits stable bluish-white electroluminescence. Studies of the perovskite material reveal three emissive contributions: a weak free-excitonic transition and two STE states (STE1 and STE2), evidencing strong electron–phonon coupling and multiple lattice-relaxation pathways. The combination of these emissive states accounts for the broadband optical response of the material. These results demonstrate the potential of 1D hybrid perovskites as single component white-light emitters and their implementation in PeLED architectures.

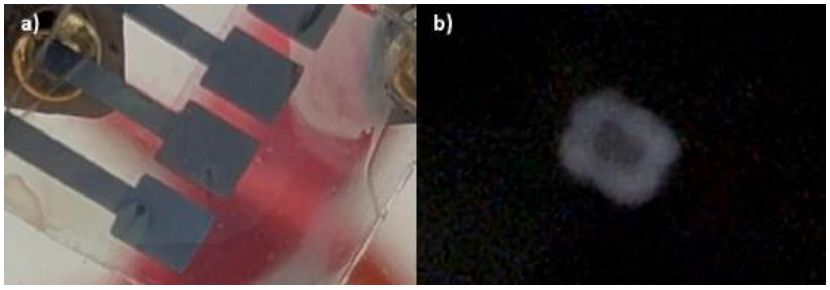

Figure 1. (a) 1D perovskite-based LED and (b) white electroluminescence from the operating device.

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Abstract preparation

THERMOANALYTICAL AND KINETIC STUDY OF PLANTAIN PSEUDOSTEM LIGNIN VALORIZATION THROUGH CATALYTIC TRANSFER HYDROGENATION

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Agricultural residues represent an important renewable resource for the sustainable production of value-added chemicals. Lignin, an abundant aromatic biopolymer, has attracted increasing attention as a feedstock for the production of phenolic compounds through catalytic conversion processes [1], [2], [3]. This work investigates the valorization of lignin extracted from the pseudostem of plantain *Musa AAB* Simmonds (Dominico-Hartón) through catalytic transfer hydrogenation (CTH), focusing on phenolic compound formation, reaction kinetics, and thermal behavior.

Lignin was extracted following ASTM D1106 using Soxhlet extraction with an ethanol–toluene mixture and sulfuric acid treatment [4]. The extraction yielded 25.5 wt% lignin relative to dry biomass. CTH reactions were performed using $NiCl_2 \cdot 6H_2O$ as catalyst precursor and an ethanol–water mixture (1:1 v/v) as solvent and hydrogen donor. A central composite response surface design evaluated reaction time (1–8 h) and temperature (25–240 °C), while total phenolic compounds were quantified using the Folin–Ciocalteu method.

The statistical model identified an apparent optimum at 25 °C and 4.82 h; however, neither reaction time nor temperature showed statistically significant effects at the 95% confidence level. FT-IR analysis revealed increased intensities of characteristic bands associated with phenolic functional groups after CTH, consistent with the formation of phenolic derivatives. The comparative FT-IR spectra are shown in Figure 1**.** Kinetic analysis under the optimized conditions showed the best fit to a pseudo-first-order model, with an apparent rate constant of 4.8792×10^{-6} s^{-1} [5].

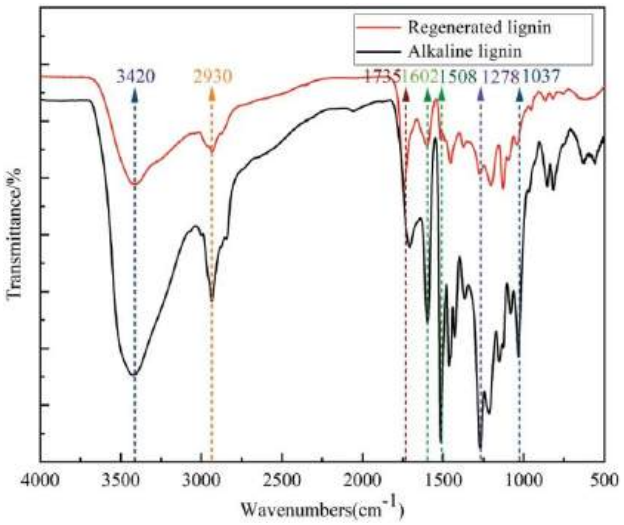

Figure 1. Comparative FT-IR spectra of untreated lignin and lignin after catalytic transfer hydrogenation under the apparent optimum conditions [5].

Thermal characterization by DSC/TGA revealed a glass transition temperature (Tg) of 150 °C**,** a recrystallization peak at 455 °C with an enthalpy of 630.4 J g^{-1}**,** and a melting peak at 718 °C with an enthalpy of 8602.4 J g^{-1} [5]. These results highlight the potential of plantain pseudostem lignin as a renewable precursor for the production of value-added phenolic compounds through sustainable biomass valorization processes.

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Range-separated MLFF with explicit intra and intermolecular decomposition for methane

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The accurate description of the Potential Energy Surface (PES) is essential for properly reproducing the dynamic and thermodynamic properties of molecular systems. However, *ab initio* methods provide high accuracy at a high computational cost, whereas classical force fields allow for extensive simulations but with lower fidelity. Machine learning force fields (MLFFs) provide an alternative by approximating quantum-mechanical potential energy surfaces at a significantly reduced computational cost.

In this work, we propose the development and evaluation of a hybrid machine-learning-based force field with a two-level decomposition. At the first level, the PES is decomposed into intramolecular and intermolecular contributions using machine learning models (sGDML). At the second level, the intermolecular contribution is further decomposed according to the interaction range. The strategy combines a short-range potential (ZBL), a machine-learning model for intermediate-range interactions (sGDML), and a long-range dispersion expansion. By doing this, a better description of the PES is sought by using different predictors, each suited to a different interaction scale. The model is implemented in molecular dynamics simulations using Python and the Atomic Simulation Environment (ASE) library to assess its performance in describing molecular configurations and its ability to reproduce relevant macroscopic properties, such as the phase diagram of methane.

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MEETING ENERGY NEEDS AS ELEMENTS FOR A JUST ENERGY TRANSITION: A CASE STUDY IN MICHOACAN, MEXICO

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Energy is fundamental to meeting human needs. However, primary energy resources come mostly from fossil fuels, which generate environmental and socioeconomic problems. Among these problems are climate change and inequality in access to energy services, especially in rural communities. Furthermore, rural communities generally bear the brunt of the environmental burdens in energy project development, without their needs being taken into account. Therefore, it is crucial to propose projects that address the energy needs of rural communities while also considering an approach to energy justice. This paper presents a case study of a project aimed at meeting energy needs in a rural community in Mexico, which considers elements that can promote greater energy justice. The study reveals a marked increase in residential energy consumption in the community compared to the public and productive sectors, where firewood accounts for more than 90% of energy consumption [1]. This aligns with the community members' perception that cooking is their most significant energy need. The main technologies implemented to address the community's priority needs were improved cookstoves, biodigesters, and photovoltaic systems for lighting and to provide electricity. The main challenges were community participation, the need for technical training, the lack of specialized technical personnel within the community, the quality of the technologies' manufacturing, and technologies high costs. It is hoped that the experience gained will contribute to the design of better projects aimed at meeting rural energy needs at both the regional and global levels.

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Acknowledgements (10 pt)
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Abstract preparation

CRYSTALLINE DYSPROSIUM OXALATE FOR OPTICAL AMPLIFICATION AT 1310 nm

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Rodolfo E. López[1], Karla Herrera[1], Grethell G. Pérez[1], Esmeralda L. Martínez[2], Ana K. Bobadilla[3], Iván Aldaya[4], Dulce Medina[5], Roberto Escudero[3]

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The growing demand for optical transmission capacity has motivated the exploration of amplification technologies beyond the conventional C-band. In particular, the O-band around 1310 nm presents attractive characteristics for optical communications due to the near-zero chromatic dispersion of standard silica fibers [1, 2]. However, suitable active optical media operating in this spectral region remain limited. In this work, crystalline dysprosium oxalate is investigated as a potential active medium for O-band amplification. Single crystals were synthesized using the modified single-diffusion gel technique and characterized by XRD, TGA, FTIR spectroscopy, and UV-Vis-NIR absorption spectroscopy. These analyses confirmed the formation of the crystalline compound and provided insight into the thermal stability, vibrational characteristics, and absorption behavior in the vicinity of the 980 nm pump wavelength. Pump-induced signal enhancement was evaluated through steady-state wavelength-resolved pump-probe measurements employing optical excitation at 980 nm and a probe signal centered at 1310 nm. The signal enhancement coefficient exhibited a clear pump-dependent increase, reaching approximately 12.0±1.7dB/mm at the highest available pump power. These results provide the first experimental observation of pump-induced signal enhancement in dysprosium oxalate single crystals and support further investigation of this material for potential O-band optical amplification applications.

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DESIGN AND CHARACTERIZATION OF NANOCELLULOSE–SILICATE HYBRID MATERIALS FOR BIOMEDICAL APPLICATIONS

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Abstract

In recent years, scientific advances in biomaterials have enabled the development of functional materials for biomedical applications in which metallic alloys and synthetic polymers are commonly utilized. However, these materials have several drawbacks: long-term wear, adverse biological responses, limited integration with biological tissues, and environmental impact of their manufacturing processes. Hence, there is a growing need to develop materials with enhanced mechanical performance, biocompatibility, and tailored functional properties while incorporating sustainable manufacturing approaches. In this study, we developed a hybrid material nanocellulose-silica supported in a poly(vinyl alcohol) (PVA) matrix. The nanocellulose was obtained from local organic waste, providing a sustainable reinforcement phase. In this composite, silica contributes bioactive properties to the material and promotes interactions with biological tissues. Incorporating both phases into the PVA matrix improves the mechanical strength, flexibility, structural stability, and overall performance of the hybrid material [1–2].

The hybrid material was synthesized using a hydrothermal method assisted by an ultrasonic transducer. The resulting material was characterized by IR spectroscopy, X-ray diffraction, TGA, scanning electron microscopy, and mechanical testing. The characterization allowed us to identify the functional groups associated with nanocellulose and PVA, as well as the Si–O–Si bonds related to the silica phase, confirming the interactions between the organic and inorganic components. The material exhibited a moderately homogeneous distribution of nanocellulose and silica within the PVA matrix. The strength, flexibility, and structural performance of the hybrid material, as evidenced by mechanical characterization, corroborate its potential for skin tissue engineering and cutaneous biomedical applications. This study evaluated the phytotoxic effects of the hybrid material on lentil (Lens culinaris) seeds.

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Abstract

DECIPHERING THE ANTIBACTERIAL AND CYTOTOXIC EFFECTS OF 1DZnO NANOPLATFORMS

Shirlley E. Martínez Tolibia[1], Rafael A. Salinas Domínguez[1], Citlaly Gutiérrez Rodelo[2], Laura J. García Barrera[3], Andrés Navarrete Castro[2], Ateet Dutt[1]*

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From the last decades, ZnO-based nanomaterials have exhibit great potential, wide versatility, and diversified physico-chemical properties to be incorporated in different applications involving biological systems. Such properties are size, morphology, nanostructural defects, synthesis methods, isoelectric point, and surface-to-volume ratio which can determine their functionality across various systems. For instance, morphologies of ZnO nanomaterials, such as nanoparticles (NPs), nanorods (NRs), tetrapods, and nanowires (NWs) seem to play an interesting role in cell-nanomaterial interaction, which require targeted characterizations.
In this work, we performed independent experiments to test the antibacterial activity of ZnO NWs against Gram-negative bacteria, and biocompatibility after interaction with mammalian cells.
The experimental setup of the antibacterial behavior was evaluated through the agar diffusion method, where ZnO NWs were placed up-side at the center of agar plates.
According to our results, moderate antibacterial activity of raw ZnO NWs was confirmed by the presence of inhibition halos against ampr-E.coli, providing updated behavior on the effects of nanowires interaction with bacterial membranes. Contrastingly, biocompatible interactions with HEK-293 cells were observed, demonstrating that ZnO NWs did not affect the substrate surrounding cells, thereby preserving morphological characteristics and viability rates, suggesting a stable bioavailability under direct contact with HEK-293. Novel nanotechnological approaches are needed to explore not only the ability to inhibit bacterial growth but also to ensure that their development is suitable for further *in vivo* assays, and effective in the long term [1].
These results provide reference for further fabrication of eco-friendly biosensing devices based on ZnO NWs, which could represent a sustainable innovation for high-throughput detection.

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High-Performance CdTe Solar Cell Incorporating Spiro-OMeTAD as Hole Transport Layer

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This work presents a novel approach to improving the performance of CdTe-based photovoltaic devices through the incorporation of Spiro-OMeTAD as a hole transport layer (HTL), employing SCAPS-1D simulation software. The proposed architecture, FTO/CdS/CdTe/HTL/Au:Cu, demonstrates a significant enhancement in power conversion efficiency (PCE), achieving a maximum value of 23%. This performance improvement is primarily associated with the optimization of the CdTe absorber layer thickness, along with the implementation of Spiro-OMeTAD as an efficient HTL.

A comprehensive qualitative and quantitative analysis of the material properties of each layer is carried out to evaluate their influence on the optoelectronic behavior of the device. The reduction in the CdTe absorber thickness not only contributes to higher efficiency but also promotes material cost reduction, which is crucial for large-scale deployment. Furthermore, the use of Spiro-OMeTAD in CdTe-based solar cells is identified as a promising alternative to conventional HTLs, due to its favorable charge transport properties and its ability to mitigate recombination losses.

Additionally, the simulation results explore the impact of key parameters within both the absorber and HTL layers, offering valuable insights into optimization strategies for device performance. Overall, the findings highlight the potential of innovative thin-film photovoltaic designs that balance reduced material consumption with enhanced efficiency.

Engineering PDMS/PVA Interpenetrating Polymer Networks through MBAAm for Skin-Like Flexible Electronic Substrates

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In recent years, stretchable, conformable, adhesive matrices have gained substantial attention due to their potential applications in soft robotics, flexible electronics, and biomedical sensors [1]. However, fabricating materials that mimic human skin with high-performance properties remains a challenge [2]. In this study, we aim to shorten this gap by examining the fabrication and characterization of interpenetrating polymer networks (IPN) that combine hydrophobic polydimethylsiloxane (PDMS) and hydrophilic polyvinyl alcohol (PVA) at various weight ratios, improving phase compatibility with methylenbisacrylamide (MBAAm). Structural, morphological, and thermal analysis (XRD, FTIR, SEM, TGA, and DSC) revealed that MBAAm suppresses crystallinity and establishes stabilizing intermolecular hydrogen bonds between PDMS and PVA [3]. These bonds minimize phase separation in the material, leading to a more uniform microstructure exhibiting gradual thermal degradation profiles, while preserving the thermal features of both polymers. Namely, PDMS/PVA IPNs are thermally stable up to 200 °C, making them suitable for deformable electronic devices working below this limit. Furthermore, mechanical tensile testing validated that MBAAm acts as a plasticizer, reducing tensile stress while maintaining high deformability (up to ~180%). The Young modulus of these materials (about 0.007-0.02 MPa) is in the same order of magnitude as the skin. Finally, EIS demonstrated a stable, predominantly capacitive dielectric response, establishing these tailored polymer matrices as a robust baseline substrate for future flexible electronics applications.

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Electrically controlled ultra-broad reflective optical bands in graded pitch bi-chiral photonic structures

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We theoretically studied the optical spectra of bichiral photonic media with a spatially varying pitch, where the optical band can be electrically controlled. The medium consists of two structurally chiral layers with opposite handedness and a pitch that varies linearly along the structure. The material possesses local $\bar{4}2m$ point group symmetry and exhibits the Pockels effect, allowing the optical spectra to be controlled via a low-frequency electric field applied along the axis of inhomogeneity; we analyzed both normal and oblique illumination. The transfer matrix method is used alongside a piecewise uniform approximation to compute the transmittances and reflectances. In the absence of an electric field, the spectra display an ultra-wide reflective band that transmits nearly all of the incident light. However, reflection increases as the electric field magnitude increases, as long as the pitch gradients of both layers are identical. The optical band edge wavelengths are expressed analytically in terms of the medium parameters and the external electric field magnitude, enabling the selection of the operating spectral region. Depending on the boundary pitch values within the layers, the band can span the entire visible spectrum. The external electric field broadens the optical band and increases the reflection of incident light up to approximately 90%. Besides, under oblique illumination, the band blueshifts as the incidence angle of light increases. Hence, these media offer potential applications as ultra-broad band reflective filters or smart windows with electrically controllable light transmission.

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Carlos G. Avendaño acknowledges financial support from the CCyT UACM under grant UACM CCYT-2026-CON-11.

$BaTiO_3$-polymer composite for piezoelectric energy harvesting: influence of polymer matrix on mechanoelectrical performance

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Ceramic–polymer composites can combine the high piezoelectric response of some ceramics with the flexibility and processability of polymers, leading to improved mechanical properties and piezoelectric performance. These materials have emerged as promising candidates for applications such as biomedical implants, self-powered systems, and energy harvesting devices. In this work, barium titanate (one of the most widely studied lead-free piezoelectric ceramics) was synthesized via wet chemical route. The effects of the titanium precursor, pH, and synthesis temperature on the final structure, as well as their correlation with electrical properties, were investigated using X-ray diffraction (XRD), Rietveld refinement, scanning electron microscopy (SEM), and multiferroic measurement techniques.

Subsequently, the optimized ceramic was incorporated into polymer matrices with either piezoelectric (PLA) or elastomeric (SEBS) characteristics, and composite films were fabricated using the doctor blade technique. The viscoelastic properties of the polymers and their influence on the piezoelectric response of barium titanate were evaluated under cyclic compression–decompression conditions using square samples (1.5 × 1.5 cm^2). The results indicate that SEBS enhances the flexibility of the composite, enabling more efficient transfer of mechanical deformation to the ceramic phase and reducing the response time compared to PLA-based composites. In contrast, the PLA matrix increases the open-circuit voltage (Voc), reaching up to 400 mV under an applied load of 10 N, whereas SEBS-based composites reached up to 170 mV under the same conditionst.

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AGROINDUSTRIAL WASTE VALORIZATION FOR FUNCTIONAL MATERIALS DEVELOPMENT AND WATER REMEDIATION IN THE PURÉPECHA REGION

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Abstract

Michoacan, Mexico is a major agroindustrial state and a national and intenational leader in mango and avocato production. However, these activities entails a substantial organic waste generation, since skin and seed represent about 20-35% of the fruit weight. Michoacan is also a producer of wood-based products such as furniture or handcraft, whose waste represent another source of organic biopolymers. At the same time, there is an increase in water stress and decline in water quality. This is particularly worse in rural areas, in which acces to safely water managed water remains a key problem. These imply two main challenges: access to safe water (in Mexico only 43% has access to water free from contaminants [1]) and waste management.

This work present biomaterials synthesized from locally available biomass, including avocado, mango, lemon, and sawdust waste. Their application as activated carbons and supporting matrices for nanocatalysts is evaluated for wastewater, residual water, and rainwater remediation. Materials and systems were tested using samples collected in communities of the Purépecha region of Michoacán under real operating conditions [2-4]. In addition, biomatrices incorporating Fe^{2+} ions were evaluated for Fenton-like catalytic reactions aimed at pollutant degradation. We discuss their application to address local rural issues that represents an oppotunity to improve the water quality (with all implicataion it has on other sectors) and a change toward new sustainable development.

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Janet Morales (1063471), K. Murguía (1271561) and S. Orozco (I1200/320/2022-I1200/331/2023/MOD.ORD.12/2025) acknowledge SECIHTI. Authors acknowledge Projects UNAM-DGAPA-PAPIIT IT100925, UNAM-DGAPA-PAPIME PE105925, and SECIHTI PEE-2025-G-104.

Tumble test study of nickel-coated steel for tribology analysis

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The materials used in daily life are constantly subjected to friction and impact with everything they are stored with, including coins, keys, and even clothing (denim and leather being the most common). Therefore, environmental and climatic conditions cause secretions from the skin, which, through the fabrics that make up clothing, come into contact with the materials of the coins, altering the pH conditions and potentially affecting their wear

The Tumble test is used to evaluate the structural integrity and mechanical resistance of handheld consumer products and materials by simulating the repeated drops, jolts, and impacts they may encounter during their lifetime. It involves rotating the product in a container to check for mechanical failure, cracks, or damage. The test uses a barrel with polygonal geometry mounted on a rotary motion device, designed to create a repeatable environment for random drops among all the components inside it. The Tumble test is versatile because it provides a simple and effective way to simulate the wear and tear that metal parts experience in real life. When metal objects or coated components are in use, they are constantly rubbing, hitting, and moving against other surfaces. The Tumble test recreates these conditions in a controlled environment by subjecting the samples to repeated friction and impact.

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Oxidizing Curiosity: Jamaica-Infusion Electrolytes for Aluminum Anodization

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In this work the electrochemical anodization of commercial aluminum was explored using *Hibiscus sabdariffa* infusion, commonly known as Jamaica, as an alternative electrolyte. This approach was motivated by the presence of organic acids in the plant extract, such as malic and citric acids, which have been previously associated with aluminum anodization processes [1–3]. Commercial LUMEN aluminum plates were used without prior surface treatment and anodized under fixed voltage and time conditions, varying only the concentration of the Jamaica-based electrolyte.

The study was originally developed as a science project for high school students at the Escuela Nacional Preparatoria (ENP, UNAM), aiming to introduce them to electrochemical synthesis and materials characterization. During anodization, visible surface changes and corrosion effects were observed after approximately 10 min, particularly at higher electrolyte concentrations. This behavior suggests that chemical dissolution of the anodic oxide may compete with oxide growth under more aggressive conditions [4].

Surface morphology was evaluated by scanning electron microscopy (SEM), revealing features consistent with electrochemical modification of the aluminum surface in the Jamaica-based electrolyte. In addition, a semi-qualitative analysis based on SEM images was performed to assess the relative roughness of the anodized samples. Although this work began as an educational project at the high school level, the research is continuing to better understand the role of organic-acid-based electrolytes in aluminum anodization and porous oxide formation.

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Oxidation-Driven Electronic and Optical Modulation in Silicon Nanowires

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Silicon nanowires (SiNWs) are promising materials for nanoelectronic, photonic, and sensing applications due to their tunable physicochemical properties.[1,2] Under ambient conditions, silicon surfaces spontaneously oxidize, leading to the formation of Si/SiO_x interfaces that strongly affect their electronic and optical behavior.[3] In this work, first-principles density functional theory calculations were employed to investigate the evolution of the electronic and optical properties of progressively oxidized ⟨100⟩ silicon nanowires. The results reveal a continuous reduction of the direct band gap from 2.00 to 1.17 eV as oxidation proceeds. Band structure and projected density-of-states analyses show that the valence-band edge remains dominated by Si states from the crystalline core, whereas the conduction-band minimum is strongly influenced by Si–O environments at the interface. Consequently, band-gap narrowing is mainly driven by a downward shift of interfacial conduction-band states. Oxidation also induces a progressive redshift of the optical absorption onset and a decrease in the intensity of the dielectric response. Charge-density analyses demonstrate that the electronic redistribution associated with oxidation is highly localized at the Si/SiO_x interface. These findings identify the interface as the key region controlling the electronic structure and optical response of oxidized silicon nanowires, providing insights for the design of silicon-based optoelectronic and sensing devices.

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DEVELOPMENT OF Ga-DOPED TiO_2 PHOTOCATALYSTS SUPPORTED ON COMMERCIAL GLASS FOR WATER REMEDIATION

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Abstract

Research and development of photocatalytic technologies has accelerated in response to declining water quality and increasing water scarcity. Key challenges include improving solar-radiation harvesting through reactor configuration and material optical properties [1], as well as developing feasible systems for scaling up to real wastewater-treatment plants.

TiO_2 is among the most widely used photocatalysts because of its redox properties, low toxicity, low cost, and high stability. However, its wide band gap requires ultraviolet activation and its rapid electron–hole recombination limits photocatalytic efficiency. In this work, TiO_2 was Ga-doped and synthesized by an ultrasound-assisted acid peptization method [2]. Recovered gallium liquid metal was used as the precursor for gallium doping [3]. To facilitate catalyst recovery, the material was supported on commercial glass, providing a fixed configuration and enabling synthesis at lower temperatures. The materials were characterized by FTIR, XRD, Raman spectroscopy, and SEM. Their photocatalytic activity for the degradation of the emerging pollutant ibuprofen was evaluated.

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COMPETITIVE ADSORPTION OF HEAVY METALS IN SYNTHETIC AND BIOLOGICAL MICELLES: A MOLECULAR DYNAMICS APPROACH

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Heavy metal contamination presents a significant environmental challenge, requiring efficient and sustainable remediation strategies. In this study, we use molecular dynamics (MD) simulations to evaluate and compare the performance of synthetic sodium dodecyl sulfate (SDS) and biological Rha-C10-C10 rhamnolipid micelles in removing divalent heavy metals, specifically Cd^{2+}, Co^{2+}, Ni^{2+}, and Zn^{2+}. Computational models were constructed, and the Radial distribution functions, charge density profiles, and intrinsic electric fields were computed to elucidate the binding mechanisms at the micelle-water interface. Our results demonstrate distinct competitive binding affinities, notably highlighting the specific anomalous radial distribution peak of nickel, as well as the strong coordination behavior of cobalt ions with the micellar polar heads. These atomistic insights provide a fundamental understanding of how biosurfactants can serve as eco-friendly alternatives to traditional synthetic surfactants for heavy metal remediation in wastewater treatment.

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ZnO Nanowires for optical biodetection of multidrug-resistant E. coli.

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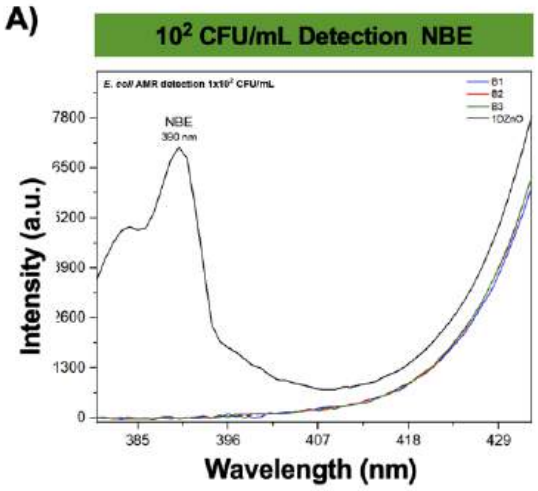
Medical treatment innovations coupled with nanotechnology have resulted in great advancements for bioimaging, drug-delivery, gene therapy, personalized medicine, pathogen biosensing, among others. This synergy has been successful due to the advantages provided by nanomaterials such as small size and morphologies, large surface-to-volume ratio, and ease of surface modification to increase biocompatibility, which have promoted an enhanced interaction with cells at intracellular and extracellular levels. Antimicrobial resistance (AMR) is a global phenomenon that has strongly impacted on the health of humans, animals, and ecosystems, which can end up in a huge pandemic outbreak in the upcoming future. In this regard, taking advantage of the luminescent properties of 1DZnO as biosensing nanoplatforms for pathogen detection, we performed experiments for detection of AMR E. coli (ampicillin and erythromycin resistant), providing increased functionalities of nanowires. First, the biofunctionalization of NWs by hydroxylation and subsequent silanization using APTMS was carried out, as reported previously. Then, polyclonal antibodies against E. coli were used to promote the immobilization of these bioreceptors over functionalized 1DZnO, placed in contact with antibody solutions (50 µg/mL). Biofunctionalized substrates were used for fast detection of multidrug-resistant E. coli, from bacterial dilutions adjusted at 10^4 CFU/mL and 10^2 CFU/mL, establishing short contact times (10 s ±2) between substrates and bacterial samples. 1DZnO substrates were washed three times in 500 µL sterile water, and PL spectra observed the presence of attached bacteria. Photoluminescence detection was performed by triplicate, and statistical analyses evaluated the obtained spectra from each concentration to characterize the specificity of the optical response and the differences between both concentrations detected of AMR E. coli. After contact with bacterial cells, it is observed an interference with the optical response, derived from the biological components from bacterial membranes such as phospholipids, porins, peptidoglycans, etc. involved in the quenching of the PL signal, a behavior that is observed both at $1x10^4$ and $1x10^2$ CFU/mL. This profile is consistent in all tested 1DZnO nanoplatforms and their replicates (B1, B2, and B3), corroborating that the peak area from NBE presents a prominent decrease, also observed in DLE, that are inversely proportional to the detected concentration



Keywords: E. coli, Biodetection, AMR bacteria

DEVELOPMENT OF NOBLE-METAL-FREE NiFe–Zn CATALYSTS FOR ALKALINE MEMBRANE ELECTROLYZERS FOR THE EFFICIENT PRODUCTION OF GREEN HYDROGEN

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Green hydrogen, a key clean energy vector for sustainable transitions, offers high energy density and zero-carbon conversion for mobility and industries like ammonia production [1]. While alkaline water electrolyzers (AWEs) enable scalable, low-cost production from renewable energy sources, the oxygen evolution reaction (OER) remains a bottleneck [2]. Thus, noble-metal-free electrocatalysts with high activity, stability, and cost-effectiveness are essential [3]. Here, we synthesized NiFeZn oxyhydroxides (NiFeZnOOH) with 1–10 at.% Zn doping (relative to Fe) via diffusion-limited aggregation electrodeposition and ultrafast ion exchange on nickel foam (NF). SEM revealed hierarchical dendritic NiO nanostructures with high surface area and porosity, optimizing active sites and electronic properties upon Fe/Zn incorporation. In 1 M KOH, the optimal composition delivered low overpotential, Tafel slope, and ≥100 h durability at 50 mA cm^{-2}, surpassing RuO_2 benchmarks. These findings position Zn-doped NiFeOOH/NF as a scalable anode for AWE-based green hydrogen production.

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Abstract

DECIPHERING THE ANTIBACTERIAL AND CYTOTOXIC EFFECTS OF 1DZnO NANOPLATFORMS

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From the last decades, ZnO-based nanomaterials have exhibit great potential, wide versatility, and diversified physico-chemical properties to be incorporated in different applications involving biological systems. Such properties are size, morphology, nanostructural defects, synthesis methods, isoelectric point, and surface-to-volume ratio which can determine their functionality across various systems. For instance, morphologies of ZnO nanomaterials, such as nanoparticles (NPs), nanorods (NRs), tetrapods, and nanowires (NWs) seem to play an interesting role in cell-nanomaterial interaction, which require targeted characterizations.
In this work, we performed independent experiments to test the antibacterial activity of ZnO NWs against Gram-negative bacteria, and biocompatibility after interaction with mammalian cells.
The experimental setup of the antibacterial behavior was evaluated through the agar diffusion method, where ZnO NWs were placed up-side at the center of agar plates.
According to our results, moderate antibacterial activity of raw ZnO NWs was confirmed by the presence of inhibition halos against ampr-E.coli, providing updated behavior on the effects of nanowires interaction with bacterial membranes. Contrastingly, biocompatible interactions with HEK-293 cells were observed, demonstrating that ZnO NWs did not affect the substrate surrounding cells, thereby preserving morphological characteristics and viability rates, suggesting a stable bioavailability under direct contact with HEK-293. Novel nanotechnological approaches are needed to explore not only the ability to inhibit bacterial growth but also to ensure that their development is suitable for further *in vivo* assays, and effective in the long term [1].
These results provide reference for further fabrication of eco-friendly biosensing devices based on ZnO NWs, which could represent a sustainable innovation for high-throughput detection.

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Session 3. Advanced Inorganic Materials

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Annealing Impact on Emission Spectra of rare earth Pr^{3+} ions in Si-rich HfO_2 films for optoelectronics applications

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Hafnium oxide (HfO_2) is technologically important material due to its attractive optoelectronic properties. The large band gap of HfO_2 (≈ 5.8 eV) and significant transparency in the wide spectral range promised its use as a matrix for light emitting elements, such as rare earth (RE) atoms. The RE atoms applications in photonics and optoelectronics related to the active-planar waveguides, energy converters for solar cells, optical fiber and amplifiers, solid state lasers and light emitting diodes, sensors and other optoelectronic devices. In this work the impact of high temperature annealing at T_a of 800-1100°C on photoluminescence (PL) via 4f shell levels of Pr^{3+}ions, as well as peculiarities of their excitation in Si-rich HfO_2:Pr films are studied. For effective emission via 4f shell levels in Pr^{3+}ions, it is important to ensure the transfer of excitation energy from matrix HfO_2 defects or Si quantum dots (QDs) to the RE ions. This work is aimed at studying the influence of T_a on the nature of host HfO_2 defects, on $Pr3^{+}$emission efficiency and PL emission spectra in Si rich HfO_2:Pr nanocrystal (NC) films obtained by the magnetron sputtering method.

The surface morphology was monitored by scanning electron microscopy (SEM), the film composition was studied by energy-dispersive X-ray spectroscopy (EDS) and high-resolution photoelectron spectroscopy (HR-XPS), the crystal structure by X-ray diffraction (XRD), as well as the visible and infrared photoluminescence (PL) spectra were controlled.

It has been shown that in highly oxidized films annealed at 1000°C, the PL excitation of low energy PL bands in the 4f shell of Pr^{3+}ions dominates. The latter is due to the involvement in the excitation of Pr^{3+}ion emission of oxygen related defects (interstitial O_i atoms and molecules). On the contrary, upon annealing at 1100°C, the content of oxygen atoms in the films decreases together with the generation of oxygen vacancies. This latter conclusion was confirmed by the analysis of the variable signals of Si2p, Hf4f, O1s and Pr3d in the high-resolution X-ray photoelectron spectra (HR-XPS) of the films. Moreover, the appearance of oxygen vacancies upon annealing at 1100°C stimulates the drastic variation of the PL spectra of Pr^{3+}ions due to the change of dominated defects, which participate in the excitation of Pr^{3+}ion emission. In the latter case, the excitation of high energy PL bands in the 4f shell of Pr^{3+}ions occurs with the excitation energy transfer through O vacancies. The results obtained are important for applications of HfO_2:Pr films in telecommunication technology.

Green synthesis of silver nanoparticles using *Clinopodium macrostemum* extract for the development of plasmonic biosensors

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Water contamination by Hg^{2+}, Pb^{2+}, and Cu^{2+} ions represents an environmental and public health risk because of their persistence and bioaccumulation. Although atomic absorption spectroscopy and inductively coupled plasma mass spectrometry provide high sensitivity, their infrastructure requirements hinder *in situ* monitoring. Silver nanoparticles (AgNPs) offer a promising platform for plasmonic sensors because their interaction with metal ions can modify particle aggregation and the surrounding dielectric environment, producing colorimetric changes associated with localized surface plasmon resonance [1,2]. In this study, AgNPs were synthesized and characterized through a green route based on an aqueous extract of *Clinopodium macrostemum* (nurite), as a first step toward the development of a heavy metal sensor. Fresh leaves were washed, shade-dried, and ground; 3 g of plant material was then infused in 100 mL of distilled water at 60 °C for 30 min and filtered. The extract was added dropwise to a 1 mM $AgNO_3$ solution at a 1:9 (v/v) ratio under stirring at 70 °C for 30–60 min. AgNP formation was evaluated by UV–Vis spectroscopy, scanning electron microscopy, and energy-dispersive X-ray spectroscopy. The UV–Vis spectrum showed an absorption maximum at 401.32 nm, attributed to surface plasmon resonance. Particle-size analysis revealed a predominant distribution between 10 and 20 nm, with an approximate mean diameter of 15 nm. The micrographs showed mostly semispherical particles, while the energy-dispersive spectrum displayed the silver L_α signal at 2.98 keV; elemental mapping confirmed the concentration of silver in the higher-contrast clusters. These findings indicate that the reducing compounds present in nurite enable the production of AgNPs with controlled size and well-defined optical properties while reducing the use of toxic reagents. Future work will quantify the plasmonic shift in the presence of Hg^{2+}, Pb^{2+}, and Cu^{2+}, and will evaluate selectivity, detection limits, and performance in different aqueous matrices.

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ABSTRACT

Synthesis and Evaluation Photoluminescent of $NaYF_4:Er^{3+}/Yb^{3+}$ Nanocrystals

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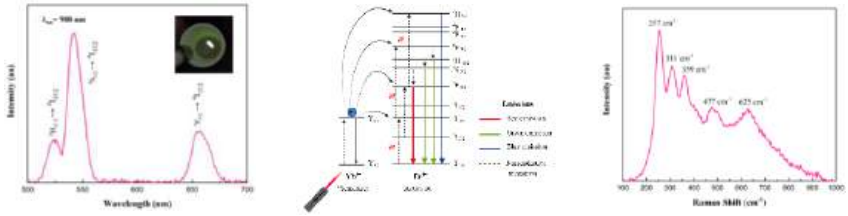
This work reports the synthesis of β-$NaYF_4:Er^{3+}/Yb^{3+}$ nanocrystals obtained through the thermal decomposition method. The resulting nanocrystals were subsequently characterized using Raman spectroscopy, FTIR, UV-Vis, DLS, and TGA to evaluate their structural properties. Their optical properties were evaluated by photoluminescence spectroscopy under 980 nm excitation, enabling the analysis of their upconversion behavior.

The results showed upconversion phenomenon with strong green emission, between 525 and 542 nm. These emissions corresponding to the $^2H_{11/2} \rightarrow {}^4I_{15/2}$ y $^4S_{3/2} \rightarrow {}^4I_{15/2}$ electronic transitions of the Er^{3+} ion. In 656 nm was detected a red emission, attributed to the $^4F_{9/2} \rightarrow {}^4I_{15/2}$ transition [1]. The band gap value of 2.57 eV was calculated using the Tauc method [2]. The Raman spectrum presented five bands at 257, 311, 359, 477 y 625 cm^{-1}, confirming the formation of the β-$NaYF_4:Er^{3+}/Yb^{3+}$ hexagonal crystalline phase. [3][4].

The results demonstrate that the thermal decomposition method is efficient for obtaining β-$NaYF_4{}^{3+}/Yb^{3+}$ nanocrystals with excellent upconversion emission properties. These characteristics make this material a promising candidate for biomedical applications, particularly in optical nanothermometry.



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Abstract preparation

EXPERIMENTS AND THEORY ON THE RHEOLOGY OF COMPLEX SYSTEMS.

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In this conference we present experimental results on the Rheology of complex materials and their theoretical description by a new approach named Connectivity Field Theory. To understand the flow of complex materials requieres model systems with fine experiments and constitutive models that may predict, optimistically, the basic behavior of these systems, with clear simplicity to be implemented numerically with demanding computational codes.

Giant micellar systems are model compounds which may provide experimental data to motivate their prediction by suitable analytical and computational models contained in the new theories. Under flow, the relevant relaxation mechanisms combine the breakage-reformation process of the micelles and the simulateneus polymer-like reptation mechanisms. These processes are examined under different flow situations like stress relaxation, inception of shear, large amplitude oscillatory flow, hysteresis, creep and considering yield-stress materials. The dynamics of these systems are similar to those observed in metals and ceramics, thereby allowing a generalisation to hybrid-materials description.

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CORRELATION OF Pt1@NiO SINGLE-ATOM CATALYSTS DINAMICS BY DRIFTS AND Cs-CORRECTED ELECTRON MICROSCOPY

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In single-atom catalysts (SACs) every atom serves as an active site, maximazing atomic utilization and activity, while reducing utilization of noble metals [1]. However, their practical implementation is limited by the challenges regarding the maintaining of the atomic dispersion of SACs under operating conditions and the large-scale synthesis. During working conditions, SACs tend to migrate and to agglomerate to minimize surface energy. Hence, strategies to enhance de metal-support interactions (MSI) need to be implemented for SACs stabilization to prevent catalytic deactivation [2]. Moreover, elucidating the dynamics of single-atoms under a external stimuli is of paramount for developing new stabilization strategies. In this regard, DRIFTS is sensitive to the dynamics of adosrbed species and can therefore serve as a proxy for single-atom movility, and coupled with atomic-resolution electron microscopy, an excellent correlation and elucidation of the restructuring dynamics can be provided. In this work, a straighforward modified wet-impregnation method is used for the synthesis of Pt1@NiO SACS is presented [3], and the effect of support on the restructuring dynamics and stability is elucidadted by in situ DRIFTS and atomic-resolution HAADF-STEM imaging.

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Section 3

THERMOLUMINESCENCE PROPERTY OF LITHIUM BORATE FOR RADIATION DETECTION

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In the framework of the search for suitable materials for the detection of ionizing radiation, lithium borate (LiBO) glasses have been investigated [1]. Several properties, such as non-toxicity, non-hygroscopic, and their low atomic number Z_{eff} close to that of the human tissue, make the borate a satisfactory radiation detector material. We present results on samarium, therbium-doped $Li_2B_4O_7$:Ag glasses prepared by the melting method. The thermally stimulated luminescence property, also named thermoluminescence (TL), was investigated in the borates glasses. The borates were exposed to beta radiation from Sr-90/Y-90 radioactive source. The beta dose-response dependence improved when the Sm or Tb ion was added, which may be creating new traps for electrons in the borate band gap. High fading was associated with shallow traps in the material. The broad glow curves can be explained by assuming the existence of a trapping level distribution. The maximum temperature of the glow peaks behaved unpredictably; normally, it increased with increasing dose. The general order kinetic model fitted the TL glow curves well. These findings are of importance in TL dosimetry because the borate glasses can be improved for suitable beta radiation detection.

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Hierarchical Black Silicon by Metal-Assisted Chemical Etching and Plasma Passivation: Surface Recombination Control for Photovoltaic and Biosensing Applications

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Abstract

Hierarchical black silicon (b-Si) combines exceptional light-trapping capability with a large specific surface area, making it highly attractive for photovoltaic, optoelectronic, and biosensing applications. However, the nanostructuring processes required to achieve ultra-low reflectance introduce a high density of surface states that increase surface recombination and deteriorate the electronic quality of the material. In this work, black silicon was fabricated on p-type crystalline silicon wafers through a combination of alkaline pyramidal texturing and Metal-Assisted Chemical Etching (MACE) using Ag and Cu catalysts deposited either by sputtering or chemical immersion. The influence of plasma-assisted passivation treatments using Ar, H_2, NH_3, Ar/H_2, and Ar/NH_3 atmospheres was systematically investigated as a function of plasma power and processing conditions.

Morphological, optical, and electronic properties were evaluated by SEM, FTIR, UV–Vis reflectance spectroscopy, photoluminescence (PL), Surface Photovoltage Spectroscopy (SPS), and minority carrier lifetime measurements using a Sinton WCT system. The combined pyramidal-MACE structures produced hierarchical black silicon surfaces with reflectance values as low as ~2–3% in the visible region, significantly lower than those of conventionally textured silicon. Nevertheless, the increased surface area generated by MACE reduced the minority carrier lifetime due to enhanced surface recombination. Plasma treatments based on NH_3/Ar atmospheres effectively passivated the nanostructured surfaces through the formation of Si–N and N–H related bonds, increasing minority carrier lifetimes from approximately 0.5 μs to 6–8 μs while preserving the excellent light-trapping characteristics of the material. FTIR analysis confirmed the formation of nitrogen-related passivating species and demonstrated that low plasma powers provided the most effective surface stabilization.

Finally, the compatibility of plasma-passivated black silicon with APTMS self-assembled monolayers was evaluated as a first step toward biofunctionalization. SEM observations revealed a controllable surface coverage that increased with assembly time, demonstrating the feasibility of integrating black silicon with molecular recognition layers. These results show that plasma-passivated hierarchical black silicon constitutes a versatile platform not only for high-performance photovoltaic devices but also for emerging optical and electrochemical biosensing technologies.

Mapping Composition, Phase Evolution, and Water-Remediation Performance in the Bi_2O_3-TiO_2 System

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The Bi_2O_3-TiO_2 system forms several crystalline phases including $Bi_2Ti_4O_{11}$, $Bi_4Ti_3O_{12}$, $Bi_{12}TiO_{20}$, and metastable compounds ($Bi_2Ti_2O_7$ and $Bi_{20}TiO_{32}$) whose formation and coexistence are governed by composition and calcination temperature. Ceramic powders were obtained by high-energy ball milling and solid-state reaction (400-800 °C); nearly 120 compositions were evaluated to relate composition, phase evolution, and adsorptive and photocatalytic performance toward rhodamine B (RhB) in water. XRD, Raman, SEM, TEM/HRTEM, and XPS showed that above 600 °C coupled biphasic heterojunctions form ((TiO_2/ $Bi_2Ti_4O_{11}$, $Bi_2Ti_4O_{11}$/ $Bi_4Ti_3O_{12}$, and $Bi_4Ti_3O_{12}$/$Bi_{12}TiO_{20}$) while lower temperatures leave residual α/β-Bi2O3 and anatase with incomplete transformation. Mott-Schottky, photocurrent, and photoluminescence analysis of the $Bi_2Ti_4O_{11}$/$Bi_4Ti_3O_{12}$ heterojunction (25/75 wt.%) indicated type-II band alignment, with improved charge separation relative to the individual phases. Dark-condition RhB adsorption followed the sequence $Bi_2Ti_4O_{11}$ < $Bi_4Ti_3O_{12}$ < $Bi_{12}TiO_{20}$, consistent with increasing Bi_2O_3 molar fraction, and increased as pH decreased. An α-Bi_2O_3-rich material prepared at low temperature reached 7.3 mg g-1 at pH 3 (pseudo-second-order, R2 = 0.977) and, in acidic chloride media, transformed in situ into flake-like BiOCl. The resulting BiOCl/TiO_2/$Bi_4Ti_3O_{12}$/$Bi_{12}TiO_{20}$ heterojunction combined adsorption and photodegradation, removing close to 100% of RhB over 12 cycles. The $Bi_2Ti_4O_{11}$/$Bi_4Ti_3O_{12}$ (25/75) heterojunction showed the highest photocatalytic activity among the compositions tested: complete degradation of RhB (10 mg/L) within 4 h under simulated and natural sunlight, and 99% degradation in 60 min with NaCl (3 mM) or at pH 3. EPR and scavenger experiments identified h+ and O2- as the dominant reactive species, with an additional contribution from Cl/Cl2- in the presence of NaCl. Unlike Degussa P25 (k = 54 × 10-3 min-1, remaining suspended after 24 h), this heterojunction settled within 30 min and retained more than 95% of its initial activity after six cycles over 21 days, with no detectable Bi or Ti leaching. Composition and synthesis temperature in the Bi_2O_3-TiO_2 system govern adsorption and photocatalysis differently, and their controlled combination yields ceramics that capture and degrade RhB, settle without centrifugation, and can be reused for solar-driven water treatment.

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Composition-Dependent Microstructure and Electromechanical Response of Lead-Free BCTZ–Natural Hydroxyapatite Biocomposites

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Abstract

Natural bone is an electroactive tissue whose mechanically generated electrical signals contribute to remodeling and repair [1-2]. This behavior motivates the development of lead-free “smart” implants that combine an electromechanical response with bio ceramics. In this work, biocomposites based on (Ba,Ca)(Ti,Zr)O_3 (BCTZ) and natural hydroxyapatite (HA) were prepared by mechanical activation followed by conventional sintering. Their structural, microstructural, ferroelectric, and piezoelectric characteristics were evaluated as a function of HA content.

X-ray diffraction and microstructural analysis revealed a clear composition-dependent evolution of the crystalline phases and ceramic microstructure. Low HA additions largely preserved BCTZ as the main crystalline phase, whereas HA contents above 5 wt% promoted secondary-phase formation, consistent with interfacial reactions during sintering. Ferroelectric hysteresis loops indicated that switchable polarization was retained after HA incorporation. The calculated longitudinal piezoelectric coefficient (d_{33}) varied with composition and reached a maximum of 2 pC/N for 10 wt% HA, within the range reported for bone tissue (0.7–2.3 pC/N) [1]. Overall, these findings identify HA content as a key parameter for balancing phase stability and electromechanical response, supporting the further evaluation of BCTZ–HA biocomposites for bone-mimetic electroactive applications [3–4].

Acknowledgements

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YVO_4: Yb^{3+}, Er^{3+}/SiO_2 nanocomposite as a nanothermometer

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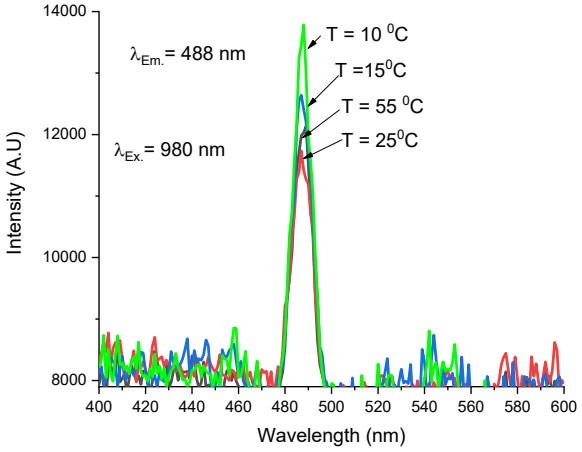
Luminescent nanothermometers leverage the photoluminescence of nanomaterials to evaluate thermal variations at the nanoscale with high spatial resolution in a non-invasive manner.

In this work, the YVO_4: Yb^{3+}, Er^{3+}/SiO_2 nanocomposite was prepared in an aqueous solution [1], in which, its optical behavior were analyzed across temperature cycles of 10, 15, 25, and 55 °C under λ_{Exc} = 980 nm.

The energy upconversion process was confirmed, characterized by an intense blue emission band centered at $\lambda_{Em.}$ =488 nm. The mechanism involves the excitation of Yb^{3+} ($^2F_{7/2} \rightarrow 2F_{5/2}$) and the subsequent energy transfer to Er^{3+}, driving the radiative transition $^4F_{7/2} \rightarrow {}^4I_{15/2}$.[2].

The spectral variations recorded as a function of temperature confirm the potential of the YVO_4:$Yb^{3+,}$ Er^{3+} /SiO_2 system for applications in high-precision optical thermometry.



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Feasibility of a Multilayer Biofilter Based on Corncob-Derived Biochar and Zeolite for Water Hardness Reduction, with Evaluation of the Biological Stability of the Lignocellulosic Material

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Abstract

Water hardness, mainly caused by Ca^{2+} and Mg^{2+} ions, affects water quality and domestic water systems. This study evaluates the feasibility of a multilayer biofilter combining corncob-derived biochar and natural zeolite for reducing the hardness of domestic tap water, while assessing the biological stability of the lignocellulosic material. Four treatments were applied to corncob: untreated material, thermal treatment, sodium hydroxide treatment, and pyrolysis for biochar production. Microbiological stability was evaluated by colony-forming unit (CFU/mL) counts, and filter performance was assessed through EDTA titration of water hardness expressed as mg/L $CaCO_3$.

The initial water hardness was **666.7 mg/L $CaCO_3$**. Biochar exhibited the lowest microbial load, with **30 CFU/mL**, compared with 80 CFU/mL for thermal treatment and 600 CFU/mL for NaOH treatment, while untreated corncob showed a count too numerous to count. Biochar was therefore selected as the optimal treatment for the multilayer filter. The biochar–natural zeolite system achieved hardness removal efficiencies of **10–50%** across the experimental runs. The first filter stage reached an average removal of **40%**, while the second reached **20%**, giving an overall average removal of approximately **30%**. These results demonstrate the potential of corncob-derived biochar as a sustainable material for domestic water treatment and agricultural residue valorization. Further optimization of material conditioning, filter configuration, and operating conditions is proposed to improve hardness removal and evaluate the reuse of spent biochar as a soil amendment within a circular economy approach.

Keywords: Biochar; corncob; natural zeolite; water hardness; lignocellulosic material; sustainable water treatment.

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One-pot solvothermal synthesis of cobalt nanoparticles supported on a cobalt microfiber network in the presence of a magnetic field.

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Cobalt magnetic microparticles and nanoparticles were synthesized via a solvothermal method using a relatively high precursor concentration of 50 mM, with oleylamine serving as the solvent. The reaction mixture was subsequently transferred to a reactor and maintained under a hydrogen atmosphere at a pressure of 10 bar for 24 h. The combined effect of the magnetic field generated by the heating/stirring plate (27.5 G) and the reaction temperature of 200 °C promoted the formation of elongated fiber-like structures and small macroscopic sheets.

Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) revealed that the fibers consisted of cobalt microparticles assembled into linear structures. Owing to the magnetic nature of the material, these arrays became intertwined, forming a network that served as a support for the cobalt nanoparticles and enabled the formation of metallic-looking sheets. These metallic sheets were stable and easy to manipulate.

Further characterization by X-ray diffraction (XRD), Raman spectroscopy, and Fourier-transform infrared spectroscopy (FTIR) confirmed that the structures were composed of pure cobalt. Atomic force microscopy (AFM) allowed the determination of the surface roughness of the nanoparticles deposited on the cobalt microparticle network. In addition, electrical resistance measurements confirmed the metallic nature of the resulting structures. This one-pot synthesis provides a straightforward route for producing homoepitaxial

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LASER ABLATION IN LIQUIDS TO PRODUCE MIXED METAL OXIDES WITH APPLICATIONS IN ENVIRONMENTAL REMEDIATION

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Abstract

Mixed Metal oxides exhibit a wide variety of crystalline structures and optical and electrical properties which make them suitable to be used in practical applications in advanced oxidation processes (AOPs). They are primarily used for water and soil decontamination due to their adsorption, reduction, and photocatalytic properties. The development of new materials basically consists of modifying the structure of matter, which can be achieved by activating chemical reactions. The generation of metal oxides can be achieved by applying electromagnetic waves to their precursor solutions, depending on the characteristics of these solutions. However, the generation of micro-/nanostructures by laser ablation is usually a bottom-up process represented by nucleation, growth and assembly of clusters from laser ablated species.

In this work, we report the synthesis and characterization of different mixed metallic oxides in thin films configurations using the laser ablation method in liquids and a study of its photocatalytic properties in the degradation of two organic colorants (methylene blue and methyl orangee

In this work, the metallic nanoparticles produced by the PLD method, were widely characterized by structural and analytical techniques. The photocatalytic studies of the degradation processes were conducted using U-V ligh and it follow-up was performed with a UV-Vis spectrophotometer. The efficiency observed in the degradation process suggesats a potential use of these materials for the degradation of organic pollutants.

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Calixarenes as Scaffolds for Well-Defined Single-Metal CO_2 electroreduction Catalysts

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Recycling CO_2 is an urgent need to mitigate a global warming, and the synthesis of added value products by using CO_2 is a strategy to incorporate it into a cyclic economy. The CO_2 reduction reaction (CO_2RR) requires catalysts at the core of development of technologies for its exploitation, and heterogenous catalysts may be the clue for large industrial applications. In this context, the design and tailoring of catalytic centers inspired by enzymatic active sites entails the development of preorganized catalysts that in the case of CO_2RR would ideally feature nearby proton donors and steric confinement around the active site.

Heterogeneous catalysts have well-known advantages over homogeneous catalysts in terms of recoverability, separation from products and enhanced stability, among others. On the other hand, homogeneous catalysis offers well-defined active sites and tunability of steric and electronic properties.

With the characteristics mentioned above in mind, we designed and synthesized homogeneous phenanthroline-appended calix[8]arene-based catalysts as well-defined sites with proximal proton donors, and heterogenized it into a carbon-nitrogen material derived from pyrolyzed aromatic cyclic isocyanurate. The preparation and characterization of the single-site heterogenized catalysts within the nitrogen doped material will be presented, together with the results of its homogeneous analogues as catalysts for CO_2RR and formation of C-C bonded compounds as deep CO_2 reduced products.

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Synthesis and Characterization of Ag-NiO Nanocomposites for Dye Degradation in Water

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The extensive use of dyes across various industrial sectors has raised growing concerns regarding their environmental impact, as they represent a major source of water body pollution. In this context, the aim of this study was to synthesize Ag-NiO nanocomposites using the alkaline salt method **[1]**, followed by chemical reduction with tannic acid acting as both the reducing and stabilizing agent **[2].** The resulting materials were characterized via UV-Vis spectroscopy and advanced transmission electron microscopy techniques, including transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM), high-resolution transmission electron microscopy (HRTEM), and energy-dispersive X-ray spectroscopy (EDS). The synthesis strategy relied on the photocatalytic properties of NiO and the ability of silver nanoparticles to enhance electron-hole pair separation and facilitate charge transfer, thereby boosting the material's photocatalytic efficiency. The photocatalytic activity of the nanocomposites was evaluated by monitoring the degradation of methylene blue dye in aqueous solution under irradiation, while their electrical properties were investigated to elucidate the relationship between electronic structure and photocatalytic performance. The results demonstrated that incorporating silver nanoparticles into NiO improves methylene blue degradation efficiency compared to pure NiO, an effect attributed to the synergy between the two components. In conclusion, Ag-NiO nanocomposites represent a promising alternative for the photocatalytic degradation of organic dyes in contaminated water, owing to their high efficiency and potential application in wastewater treatment processes.

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Sequential electrophoretic deposition of HAP/Dental Porcelain on SS-316L for biomedical applications

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Nowadays, the hydroxyapatite is one of most important materials to biomedical applications due to its chemical stability, osseoconductivity and biocompatibility[1].

Nevertheless, many coatings techniques have been performed to the preparation of hydroxyapatite[2]. However, the electrophoresis due to its efficiency, flexibility and economy is most atractive in comparision with others methods. Nevertheless, the bonding strength between the coating and metallic substrates is weak therefore post-sintering is required. The sintering process is limited by of thermal properties mismatch of materials employed.

The aim of this work, was to resolve this problematic, using a material with intermediate thermal properties between HAp and SS316L.The sequential deposition of both materials by development of intercalated layers of porcelain and HAp. The EPD was carry out at 800V at deposition time of 15s. The densification of coating was made at temperatures of 950, 900 y 850° C with a soaking time of 2 h.

The results showed that dense, homogenous and free cracking coatings with a hydroxyapatite of Ca/P ratio of 1.7 were obtained, thickness greater than 11 microns and 12.46 mg/cm^2 mass deposited. The adhesion strength of coating according to ASTM F1044-05(2017) and the results obtained showed that the adhesion strength risen with increase of the densification of coating. In this way, the maximum value for adhesion strength was upper 14 MPa.

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Quantum Dots Produced by Pulsed Laser Ablation in Liquids: A Sustainable Route Toward Advanced Functional Nanomaterials

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The development of advanced functional nanomaterials with tailored optical, electronic, and chemical properties is central to emerging technologies in energy conversion, sensing, photonics, and biomedicine. Among these materials, quantum dots have attracted considerable attention because of their size-dependent electronic structure, tunable emission characteristics, and strong light–matter interactions. However, conventional chemical synthesis methods often require complex reaction schemes, toxic precursors, and surface ligands that can limit material performance and environmental sustainability.

This plenary lecture will present pulsed laser ablation in liquids (PLAL) as a versatile and environmentally friendly platform for the synthesis of high-purity quantum dots [1] and nanostructured materials. By exploiting the extreme nonequilibrium conditions generated during laser–matter interactions, PLAL enables the direct production of ligand-free colloidal nanomaterials with clean and highly reactive surfaces. Recent advances in the synthesis of semiconductor quantum dots and related nanostructures will be discussed, highlighting the influence of laser parameters, liquid environment, and post-synthesis aging on particle size, morphology, crystal structure, and optical properties.

Particular emphasis will be placed on the relationship between nanoscale structure and functionality, including quantum confinement effects, photoluminescence behavior, charge transport, and interfacial phenomena. Examples involving chalcogenide-based nanomaterials [2] and emerging quantum materials will illustrate how laser-based synthesis can produce colloids with remarkable long-term stability while preserving surface activity. The opportunities offered by these materials for flexible optoelectronics, photocatalysis, and next-generation photonic devices will also be explored.

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DEVELOPMENT OF HIGH-PERFORMANCE RARE-EARTH-BASED MAGNETOCALORIC MATERIALS VIA SPARK PLASMA SINTERING FOR HYDROGEN LIQUEFACTION

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The efficient use of molecular hydrogen (H_2) as a clean energy vector requires its liquefaction, which occurs below 20.3 K. Magnetic refrigeration (MR), a technology based on the magnetocaloric (MC) effect, has emerged as a viable alternative in the effort to develop high-efficiency hydrogen liquefiers [1,2]. However, this requires materials with a large reversible MC response in the 77-20 K temperature range (if liquid N_2 is used for a precooling stage), that can be shaped into geometries compatible with MR devices. Despite current concerns about the cost and global supply of rare-earth (R) elements [3], heavy R-based ferromagnetic compounds, such as RX_2 Laves phases (X= Ni or Al; cubic $MgCu_2$-type structure), HoB_2 and RNi_5 (hexagonal AlB_2- and $CaCu_5$-type structures, respectively), are currently among the most promising MC substances for hydrogen liquefiers [4]. Their excellent MC properties stem from high saturation magnetization, owing to the large magnetic moments of the R elements, and moderate specific heat in this temperature range. Together, these features yield large maximum adiabatic temperature ($|\Delta T_{ad}|^{max}$) and magnetic entropy ($|\Delta S_M|^{max}$) changes [4]. In recent years, our research group at IPICyT has synthesized MC compounds from the aforementioned families by arc melting, suction casting, and rapid solidification, and consolidated powders into high-density bulks by Spark Plasma Sintering (SPS) [5-8]. This talk summarizes the main results; in all cases, the MC performance is comparable to or better than that reported for the best bulk alloys.

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Effect of A-site partial substitution in bismuth ferrite perovskites on the electrical and magnetic properties

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Bismuth ferrite ($BiFeO_3$) is one of the most studied multiferroic compounds, and it crystallizes at room temperature in a rhombohedrally distorted perovskite structure with *R3c* space group [1]. The preparation of pure-single-phase is a challenge by the narrow interval of the thermal stability and formation of secondary phases, such as, $Bi_2Fe_4O_9$, $Bi_{25}FeO_{40}$ and $Bi_{46}Fe_2O_{72}$ [2]. In the present work, it was realized the synthesis of a true pure $BiFeO_3$ phase during the partial A-site substitution by different cations (La^{3+}, Dy^{3+}, Pr^{3+}, Gd^{3+}, Eu^{3+}) using Pechini method. XRD results revealed the $BiFeO_3$ phase in all the compounds. The Rietveld refinement confirmed the rhombohedral structure (R3c space group) and the succesful formation of solid solutions. In addition, the slight variations in the cell parameters, as well as density measurements confirmed the partial substitution of Bi^{3+} by the diverse cations into the A-site of the $BiFeO_3$ crystalline structure. Scanning Eleectron Microscopy displayed the succesful grain densification with low intergranular porosity obtained in the ceramics using conventional sintering process. The electrical response of the specimens was evaluated by Electric Impedance Spectroscopy (EIS) measurements in the frequency range of 1 kHz-1MHz at different temperatures. The specimens with Pr^{3+} and La^{3+} showed higher permittivity values at the diverse frequencies in comparison with the other cations. The magnetic response of the ceramics exhibited modifications in the hysteresis courves and coercive fields in comparison with the $BiFeO_3$ compounds.Finally, the results fo this study provided interesting data attributed to the single-phase $BiFeO_3$ compounds and they mar find potential device applications.

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Abstract preparation

Structural and morphological study of La-doped ZnO nanoparticles

Fabian Mendoza Hernández[1], Erasto Vergara Hernández[2], Ana Karen Acero Gutiérrez[3], Irlanda Grisel Cruz Reyes[4], Katia Lozano[5], Fernanda Aryll Hernández Ramírez[1]

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In this study, six samples of ZnO doped with 3 wt% La^{3+} were prepared using a mechanical processing method with varying milling times (1, 3, 9, 30, 90, and 360 minutes). The nanopowders were characterized by X-ray diffraction (XRD), Raman spectroscopy, and photoluminescence (PL). Structural analysis reveals the incorporation of lanthanum ions into the ZnO crystal lattice. XRD patterns show slight shifts in the main Bragg angles as milling time increases, attributed to La^{3+} occupying vacancies within the ZnO. The mechanisms underlying the optical transitions observed in the photoluminescence spectra are analyzed and discussed.

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Relaxor behavior in $Dy_{3-x}Sc_xTaO_7$ ($0 \leq x \leq 0.15$) weberite-type system.

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Among the structural derivatives from the fluorite structure (A_4X_8) there are two widely studied structures that include intrinsic anion vacancies and share the general formula $A_2B_2X_7$: pyrochlores and weberites [1]. The weberite-type structure (A_3BX_7) is derived from the weberite with different cation ordering and further distortion of the coordination polyhedra, for oxides it is formed with trivalent (A) and pentavalent (B) cations. Many structural studies have been made on rare-earth tantalates and niobates with pyrochlore, weberite and weberite-type structures due to interest in their electrical, magnetic or catalytic properties [2-4]. However few reports have dealt with the dielectric properties of these systems. In this work, ceramic samples in the system $Dy_{3-x}Sc_xTaO_7$ with the weberite-type structure were prepared via solid state synthesis and studied through X-ray diffraction, dielectric measurements, thermal analysis and measurements of magnetic susceptibility. XRD (exemplified in Figure 1) and DSC measurements show no evidence of structural transformations between room temperature and 300 °C, while the dielectric measurements (exemplified in Figure 2) reveal frequency-dependent maxima in permittivity in this temperature range indicating relaxor bahavior in all samples, including the one with x = 0.

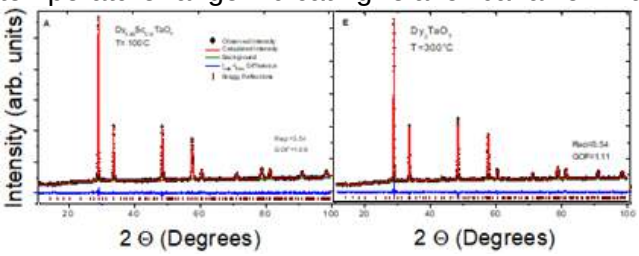

Figure 1. Rietveld plots for Dy_3TaO_7 at 100 and 300 °C.

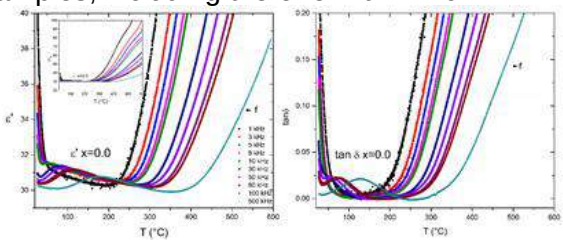

Figure 2. Temperature profiles of ε' and tanδ for Dy_3TaO_7.

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Artificial intelligence-driven design of solid solution lightweight refractory high-entropy alloys: a comparison between two quinary systems

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The lightweight refractory high-entropy alloys (LW-RHEAs) are promising candidates for advanced engineering applications because of their excellent mechanical performance and microstructural stability [1, 2]. However, reducing density while retaining favorable mechanical properties requires the efficient exploration of vast compositional possibilities under multiple design constraints [3]. In this work, an integrated computational and artificial intelligence-assisted strategy was applied to ten quinary alloy families derived from the TiVAl system and permutations of Ta, Mo, Hf, Zr, and Nb. The non-dominated sorting genetic algorithm II, thermodynamic descriptors, CALPHAD calculations, and artificial neural networks were combined to optimize density (ρ) vs bulk modulus (B). Consequently, Pareto fronts containing more than 2500 candidate compositions were generated for each family and subsequently their equilibrium phases were mapped as a function of constitution and fractions at 1100 °C. This work compares two different alloys, $Ti_{30}V_{20}Al_{30}Nb_{10}Ta_{10}$ and $Ti_{30}V_{22}Al_{28}Zr_{10}Mo_{10}$, which were fabricated by vacuum arc melting furnace and characterized by XRD, SEM-EDS, and Vickers microhardness. The former showed a dendritic microstructure and a hardness of ≈520 HV, whilst the latter exhibited a clearly segregated Laves phase and a lower hardness of ≈408 HV. These contrasting results demonstrate the potential and family-dependent limitations of AI-driven design for LW-RHEAs.

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Cooling-Rate-Induced Microstructural Evolution and Magnetocaloric Enhancement in $MnCoGeB_{0.02}$

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MnCoGe-based alloys are promising candidates for magnetic solid-state refrigeration applications [1] because their magnetocaloric response is closely related to first-order magnetostructural transitions [2–6]. The present work analyzes the relationship between microstructural evolution and the magnetocaloric response of a $MnCoGeB_{0.02}$ alloy obtained by the suction-casting technique.

The conical geometry resulted in significant cooling-rate variations along the sample axis. Variations in the cooling rate promoted different fractions of the hexagonal Ni_2In and orthorhombic TiNiSi phases, which in turn modified the magnetostructural coupling and the resulting magnetocaloric response. However, the influence of local solidification conditions on suction-cast MnCoGe alloys remains poorly understood. To investigate these effects, the conical sample was divided into different sections along its axis and subsequently characterized by structural, thermal, and magnetic techniques.

Structural characterization by X-ray diffraction and Rietveld refinement revealed the coexistence of both crystallographic phases. The relative phase fraction were strongly influenced by the local solidification conditions. Thermal and magnetic experiments showed modifications in the structural and magnetic transition temperatures, as well as in the magnetostructural coupling, depending on the microstructural variations. As a result, the magnetocaloric effect exhibited significant differences. The highest magnetocaloric response reached $|\Delta Sm(Tpeak)| = 12.3\ J\ kg^{-1}\ K^{-1}$, whereas the lowest response was approximately $|\Delta Sm(Tpeak)| = 6\ J\ kg^{-1}\ K^{-1}$. Both values were estimated under a magnetic field change of $\Delta\mu_0 H = 5.0\ T$ [7].

Different cooling rates generated during suction casting significantly modified the magnetocaloric response without changing the alloy composition. This represents an attractive alternative for developing functional materials for magnetic solid-state refrigeration applications.

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Abstract preparation

Effect of Ca and Sr Substitution on the Magnetic Transition of $La_{1-x}A_xMnO_3$ Manganites Synthesized by the Pechini Method

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The compounds with the general formula $La_{1-x}A_xMnO_3$, where A represents a divalent metal that partially substitutes for lanthanum, belong to the family of ceramics known as lanthanum manganites, which are characterized by a perovskite-type crystal structure. These materials have attracted considerable scientific interest due to the diversity of their physicochemical properties, which can be tailored through their composition and stoichiometry[1]. Among these properties are their electrical, magnetic, and structural characteristics, as well as their high chemical stability. These features make them promising for applications in the development of sensors for the detection of various physical quantities[2], magnetic devices[3], [4], [5], electrodes[6], and catalytic processes.

The present work conducts a comparative study of two lanthanum manganite compounds, in which the A-site of the perovskite structure is occupied by Ca and Sr, synthesized using the Pechini method. Particular attention is given to the effect of cationic substitution on the magnetic transition of the materials, with the aim of evaluating their potential for technological applications. The synthesized materials were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and vibrating sample magnetometry (VSM). XRD was used to determine the phases present and their structural characteristics; the morphological characterization of the samples was performed by SEM, while the Curie temperature (T_C) and the magnetic transition behavior were determined using VSM

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Synthesis and characterization of $Ba_{1-x/2}Ca_{1-x/2}Rb_xP_2O_{7-x}$ (x = 0.0, 0.05) for possible application as a solid electrolyte

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We studied the crystal structure and electrical conductivity of the mixed pyrophosphates $BaCaP_2O_7$ and $Ba_{0.975}Ca_{0.975}Rb_{0.05}P_2O_{6.95}$ to calculate activation energies for ionic transport. The aim of calculating these activation energies and determining the mechanism of ionic transport is to assess the potential application of these pyrophosphates as solid electrolytes in electrochemical devices such as proton exchange membrane fuel cells (PEMFCs)[1]. The compounds were synthesized by the Pechini citrate gel method, using the corresponding metallic carbonates and NH4H2PO4 as a source of phosphate ions. The experimental diffraction pattern showed no resemblance to the reported phases of stoichiometry $BaCaP_2O_7$ [2]. However, the mixed pyrophosphate's $BaCaP_2O_7$ structure could be refined by the Rietveld method, taking as a starting point the crystal structure of the hexagonal phase σ-$Ba_2P_2O_7$[3] (Space group $P\bar{6}2m$, No. 189). Upon addition of Rb^+ as a dopant the pyrophosphate adopted a crystal structure isostructural with the orthorhombic phase α-$Ba_2P_2O_7$[4] (Space group $Pnma$, No. 62). The presence of the pyrophosphate ion was confirmed in both compounds by identifying the absorption bands with infrared spectroscopy. Electrochemical measurements in direct current showed that pyrophosphate $BaCaP_2O_7$ has poor electrical conductivity in an anhydrous atmosphere, reflected in unusually high apparent activation energies (3.24 and 1.74 eV). In the presence of water vapor, these activation energies significantly diminish (0.60 -0.90 eV), very likely due to the presence of orthophosphate defects in pyrophosphate crystallographic positions. In sharp contrast the doped compound $Ba_{0.975}Ca_{0.975}Rb_{0.05}P_2O_{6.95}$ has a much higher electrical conductivity and exhibits lower activation energies (0.71-1.36 eV), which is explained by the presence of intrinsic *n*-triphosphate defects that react with O_2 to yield orthophosphate defects. Activation energies of this pyrophosphate decrease with increasing H_2O partial pressure in an oxygen atmosphere.

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Catalytic reduction of CO_2 with heterogeneous iron and copper catalysts

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The continuous increase in CO_2 emissions has promoted the development of strategies to convert this greenhouse gas into value-added chemicals such as methane, methanol, and ethanol. Among these strategies, thermocatalytic CO_2 reduction using heterogeneous catalysts has emerged as a promising alternative. However, the development of catalysts with high activity and selectivity remains a major challenge.[1]

In this work, we focus on synthesizing and evaluating M-N-C (metal-nitrogen-carbon) type single-atom catalysts (SACs) using iron or copper as the active metal, as these metals can yield good results at a lower cost. These catalysts were obtained through the synthesis of a zeolitic imidazolate framework (ZIF), followed by pyrolysis at 800 °C (M-1-800).[2] Various characterization techniques confirmed the presence of nanoparticles and dispersed metal atoms in these materials, both of which play a significant role in hydrogenation reactions. Their catalytic performance was evaluated in the thermocatalytic reduction of CO_2 using phenylsilane as and H_2 source [3]. Among the catalysts studied, the Cu-1-800 catalyst exhibited higher selectivity toward methanol compared to the iron-based material, suggesting that the nature of the metal plays a fundamental role in CO_2 reduction reactions.

These findings demonstrate the great potential of ZIF-derived heterogeneous catalysts for the thermocatalytic valorization of CO_2 and contribute to the development of more efficient catalytic materials for the selective production of methanol.

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MULTIFUNCTIONAL SMART INORGANIC NANOMATERIALS

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Nanomaterials have emerged as key tools in the development of innovative formulations within materials, construction, wood treatment, cosmetic and pharmaceutical industries and for use in water tratment, contaminant detection, and countless uses that have an effect on daily life.
The fact that a material is nanoparticulate changes its properties compared to the same material on a macro scale is what makes them interesting. Given its high surface/volume ratio, quantum effects become important since we are at the boundary between the laws governing the classical and quantum worlds. It is precisely this that allows us to obtain different properties by modulating the size and shape of nanomaterials[1].
We can list many types of organic and inorganic nanoparticles, and various methodologies for their preparation. Now a days it is possible to create a custom design to obtain the desired properties in the sought-after nanomaterials, based on both the type of material and its functionalization, to give it customized properties.
This presentation will explore different types of synthesis as well as various examples of industrial and environmental applications of nanomaterials, moving from additives for the cosmetics industry, wood treatment, colorimetric nanoprobes and degradation of industrial dyes.
Moving from metallic nanoparticles such as silver nanoparticles, bimetallic iron-silver core-shell nanoparticles, inorganic salt nanoparticles such as zinc borates, polymeric nanoparticles of molecularly imprinted polymer nanocomposites.[3,4]
An attempt will be made to provide an overview and present specific cases.

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FORMACIÓN DE MULLITA A PARTIR DE CAOLÍN, BOEHMITA Y UREA.

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La mullita ($3Al_2O_3 \cdot 2SiO_2$) es un material refractario de gran importancia debido a su elevada estabilidad térmica, resistencia a la corrosión, baja expansión térmica y alta resistencia al choque térmico [1]. Sin embargo, su formación a partir de caolinita involucra diversas transformaciones térmicas, entre ellas la deshidroxilación y el reordenamiento estructural, que pueden influir en las fases cristalinas obtenidas [2]. Además, la formación de mullita depende de factores como la relación Al/Si, las características de las materias primas y su reactividad durante el tratamiento térmico [3], así como de las características de las partículas de los minerales arcillosos [4]. En este contexto, el desarrollo de estrategias que permitan mejorar la formación de mullita y modificar sus características microestructurales resulta de interés para la obtención de materiales refractarios con propiedades adecuadas. En este trabajo se evaluó la síntesis de mullita a partir de caolín comercial y boehmita, empleando urea como agente de combustión. Las fases cristalinas obtenidas fueron identificadas mediante DRX y cuantificadas mediante refinamiento Rietveld. El caolín inicial presentó caolinita como fase principal, acompañada de cuarzo y cristobalita. Después del tratamiento térmico, se identificó la formación de mullita en ambos sistemas, además de fases residuales de α-Al_2O_3 y cristobalita. El refinamiento Rietveld mostró que la incorporación de urea produjo un incremento aproximado de 2 % en peso en el contenido de mullita respecto al sistema sin agente de combustión, indicando un efecto limitado bajo las condiciones estudiadas. Adicionalmente, la incorporación de urea modificó el tamaño de cristalito asociado al plano (110) de la mullita, disminuyéndolo de 273.94 nm para el sistema caolín–boehmita a 198.50 nm para el sistema caolín–boehmita–urea. Los resultados indican que el ajuste de la relación Al/Si mediante la incorporación de boehmita permite obtener mullita a 1200 °C durante 2 h. Sin embargo, la presencia de α-Al_2O_3 y cristobalita evidencia una conversión incompleta de las materias primas. Asimismo, aunque la urea produjo un ligero incremento en la cantidad de mullita, su efecto sobre el rendimiento fue limitado; no obstante, modificó el tamaño de cristalito de la fase formada. Por lo tanto, se requiere optimizar la composición de los precursores y las condiciones de combustión para favorecer una mayor conversión hacia mullita y reducir la formación de fases residuales.

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SHAPE-DIRECTED SYNTHESIS OF METALLIC NANOPARTICLES: CONTROLLING GROWTH AND STRUCTURE

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The final shape and structure of a metallic nanoparticle are established during nucleation and growth, when even small changes in reaction conditions can lead to very different outcomes. The crystallographic structure of the seeds, precursor concentration, temperature, rate of precursor reduction, and capping molecules all affect where and how atoms are incorporated. Understanding this interplay is key to controlling particle size, composition, exposed facets, and internal defects, and therefore to tailoring optical and catalytic properties.
Au–Cu systems provide several examples of controlled overgrowth of fivefold-concave particles, producing branched nanostars whose morphology and plasmonic response depend on selective facet passivation and the presence of copper ions [1]. In a different synthesis, varying the metal-to-seed ratio, temperature, and Cu/Au ratio enabled either retention of the icosahedral seeds' symmetry or its breaking, producing triangular nanotripods with improved catalytic activity [2]. A related Ni-Pt system highlights the role of surface chemistry: PDDA acted not only as a stabilizing agent but also as a growth-directing molecule, promoting step-pyramidal structures with complex surfaces that enhanced the catalytic reduction of 4-nitrophenol [3]. In this work, we discuss how control over the growth process can yield well-defined nanostructures; this overview is achieved by using electron microscopy to link the synthesis conditions to the observed morphologies, chemical composition, and facets.

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Permanent magnets with enhanced properties obtained by SPS technique

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Permanent magnets based on RE-Fe (RE=light rare earth elements) compositions are widely employed in advanced technological applications owing to their excellent combination of magnetic properties, including high intrinsic coercivity values (between 500 – 1000 kA/m), high saturation magnetization (typically ~1.5 T or higher), and outstanding maximum energy product $(BH)_{max}$ values within the range 100 to 500 $kJ \cdot m^{-3}$ [1].Given their superior magnetic performance, significant research efforts have been devoted to exploring novel processing routes, compositional optimization strategies, and advanced characterization methodologies. In particular, considerable attention has been directed toward the development of soft/hard magnetic nanocomposites with optimized exchange coupling, aiming at the fabrication of isotropic magnets exhibiting $(BH)_{max}$ > 100 kJ/m^3. In this context, Spark Plasma Sintering (SPS) has emerged as a promising densification technique to obtain bulk magnets with optimized microstructural features ensuring an enhanced magnetic performance. This consolidation technique uses a concomitant application of pulsed electric current and uniaxial mechanical pressure that enables the consolidation of highly dense bulk samples while preserving fine microstructures. SPS has been successfully employed to fabricate a wide variety of metallic alloys with tailored properties [2]. In this work, we demonstrate that Spark Plasma Sintering enables the effective translation of the optimized microstructure of melt-spun Nd-Fe-B alloys into highly densified bulk nanocomposite magnets without significant degradation of magnetic performance. The consolidated material exhibits a coercive field of 400 $kA \cdot m^{-1}$, a saturation magnetization of 1.1 T, and a maximum energy product of 110 $kJ \cdot m^{-3}$. These competitive properties arise from the preservation of a refined nanostructure containing ~88 vol.% of the hard magnetic 2/14/1 phase, which ensures strong exchange coupling and substantial coercivity in the bulk state. Our results highlight SPS as an efficient consolidation strategy to bridge the gap between high-performance melt-spun ribbons and fully dense bulk permanent magnets, providing a viable route for the scalable fabrication of nanostructured high-performance Nd–Fe–B-based permanent magnets.

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Catalytic Hydrogenolysis of *Sargassum*-Derived Compounds over Cobalt Supported on a Nitrogen-Doped Carbon Matrix

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Sargassum spp. is a brown macroalga that has experienced an unprecedented, uncontrolled proliferation in recent years, precipitating severe environmental and economic challenges.[1] Driven by the need to mitigate this crisis, numerous strategies have been developed to valorize and utilize this biomass as a sustainable feedstock for high-value-added chemicals and advanced functional materials.[1] This work presents the hydrogenolysis of alginic acid, the main macroalga polysaccharide, along with two related biomass-derived compound, mannitol and glycerol, over cobalt catalysts supported on a nitrogen-doped carbon matrix (Co-N-C) synthesized from the Sargassum itself.[2,3,4,5] The material's architecture has been designed to optimize the selective cleavage of C-C and C-O bonds to efficiently produce glycols.[5,6] By utilizing this residual biomass as both a substrate and a catalytic support, this approach aligns with circular economy and green chemistry principles to provide a sustainable alternative to fossil-based feedstocks.[1]

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Section 3-Chavira Martínez Elizabeth

EFFECT OF $CoCl_2$ ON SOIL MICROBIAL FUEL CELLS (SMFC)

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Alternative energy sources have been extensively investigated to meet the growing global demand for sustainable and efficient energy production. Soil microbial fuel cells (SMFCs) represent a promising *in situ* bioenergy technology that exploits the metabolic activity of naturally occurring electroactive microorganisms in soil to generate electrical current. [1] In this work, we evaluate the operational stability of an SMFC under controlled Co^{2+}-induced ionic perturbation through cobalt chloride ($CoCl_2$) addition. The system was tested under four treatments (control, 50, 100, and 200 mg $CoCl_2$; n = 4 per treatment), while monitoring soil physicochemical parameters, voltage, and short-circuit current density (JSC). $CoCl_2$ addition induced transient soil acidification and increased ionic strength. Although JSC exhibited a transient amplification exceeding 300% during the early perturbation phase, the system progressively converged toward stabilized, concentration-dependent regimes with bounded variability ($CV_{late} \approx 0.21–0.29$) and minimal drift ($|slope_{late}| < 0.01$ A m^{-2} day^{-1}). Soil pH showed the strongest correlation with JSC ($\rho \approx -0.54$ to -0.68), highlighting the dominant role of proton-related electrochemical conditions under ionic stress.

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MAGNETIC RELAXATION IN Ru(III) COMPLEXES WITH TRIDENTATE AMINODICARBOXYLATE LIGANDS

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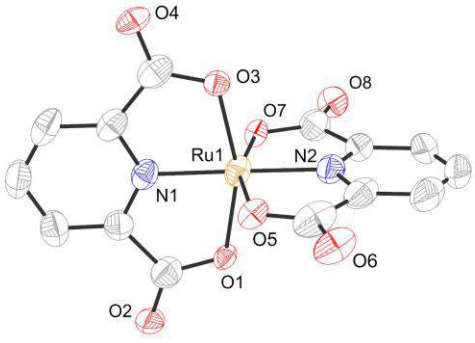
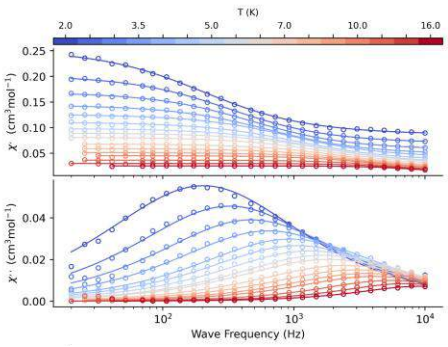
The magnetic relaxation dynamics of Ru(III) complexes remains comparatively unexplored, despite the potentially interesting properties arising from the combination of a low-spin d^5 electronic configuration (S = 1/2) and the significant spin–orbit coupling associated with this 4d ion [1,2]. Expanding the still limited number of magnetically characterized Ru(III) compounds is therefore important for establishing relationships between coordination environment, molecular and crystal structure, and spin relaxation.

In this work, we investigate the magnetic properties of two Ru(III) complexes containing aminodicarboxylate ligands, $(PPh_4)[Ru(dpic)_2]$ and $(PPh_4)[Ru(ida)_2]$ (dpic = pyridine-2,6-dicarboxylate; ida = iminodiacetate). In both compounds, the Ru(III) ion is coordinated by two tridentate ligands, resulting in closely related N_2O_4 coordination environments, while the different nature and rigidity of the ligands provide distinct molecular and crystal environments around the metal center.

Magnetic susceptibility measurements were performed to characterize their static magnetic properties and low-temperature spin dynamics. The results are presented and discussed comparatively, with particular attention to the possible influence of the coordination environment and structural differences on the magnetic relaxation of the Ru(III) centers. This study provides further experimental information on the magnetic behavior of low-spin Ru(III) complexes and contributes to the development of structure–magnetic relaxation relationships in this still scarcely explored family of molecular magnetic systems.





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KINETIC ANALYSIS OF THERMOLUMINESCENT GLOW CURVES IN SYNTHETIC POLYMINERAL MATERIAL FOR IDENTIFICATION OF IRRADIATED FOODSTUFFS

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Feldspars minerals are useful to identify the foodstuffs processed by ionizing radiation due to their enough bandgap. In particular, the anorthoclase $(Na,K)AlSi_3O_8$ with small contain of Ca, can make the whole inorganic composition of the foodstuffs [1,2]. The synthetic polymineral analogue of the inorganic compound from the commercial Mexican red paprika (*Capsicum annuum*) is analyzed using the thermoluminescence (TL) property to determine its radiation response [3,4]. The synthesis was carried out by the solid-state method with thermal annealing at 1200 °C for 6 h. The EDS elemental analysis showed the chemical composition is (wt%): O (49.4), Al (12.2), Si (29.7), Na (6.0), K (1.4), Ca (1.3). The samples were selected with <74 μm particle size and exposed to different doses from beta radiation provided by a $^{90}Sr/^{90}Y$ source. TL measurements were carried out from room temperature to 400 °C with a 2 °C/s linear heating rate. The Computerized Glow Curve Deconvolution (CGCD) of the TL glow curve was performed assuming the General Order Kinetics (GOK) model, achieving a Figure of Merit (FOM) around 2%, identifying six main peaks that well described the glow curves of the synthetic material.

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Activity Against ESKAPE Bacterial Pathogens of Pyrazole-Indol-Ruthenium(II) Complexes

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Four indole-derived iminopyrazole ligands were synthesized and coordinated with the precursor [Ru(η^6-*p*-cimene)Cl_2]. They were characterized using spectroscopic (IR, Raman, UV-VIS, NMR) and mass spectrometric (ESI-MS and IE-MS) techniques, in addition to density functional theory calculations, single-crystal X-ray diffraction (XRD) and Docking Molecular. The ligands and the resulting complexes were evaluated against resistant bacteria. The quantify antibacterial activity, the minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) of the ligands and ruthenium complexes were evaluated against six isolated bacterial strains (Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa, Escherichia coli, and Shigella dysenteriae) and two control strains: Enterococcus faecalis ATCC 29212 and Enterobacter cloacae ATCC 13047. Enterococcus faecalis and Staphylococcus aureus are Gram-positive bacteria, while the others are Gram-negative. The results were very promising, as the ruthenium complexes showed activity against resistant bacteria, including all those belonging to the ESKAPE group, a set of nosocomial (hospital-acquired) pathogens that exhibit high resistance to antibiotics. [1]

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Textural properties and rate of reduction assessment of microemulsion synthesized Cu-ZnO/Al_2O_3 catalysts

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Methanol synthesis is generally achieved by reacting CO_2 and H_2 over a Cu-ZnO/Al_2O_3 catalyst. Active site dispersion and stabillity in the catalyst are determinant of the long term catalytic activity. In this research a microemulsion based synthesis is used to control the particle size of Cu and ZnO in an attempt to increase their dispersion [1]. Reducibility of the obtained particles is studied by temperature programed reduction (TPR). Textural properties were determined using standar procedures for nitrogen adsorption (Sync 110A). TPR determinations were performed dynamically from 40 to 600 °C using 30 ml/min of H_2/Ar 10% at a heating rate of 10°C/min [2] (AMI-300Lite). The materials were synthesized using multiple techniques: (1) CR-reference catalyst prepared by coprecipitation of metal nitrates; (2) SS-simultaneous synthesis: Cu-ZnO nanoparticles synthesized via a reverse micelle-assisted route and incorporated into the alumina hydrolysis phase (sol-gel method); (3) AIS-alumina impregned with metal salts, alumina fabricated by the sol-gel technique with copper and zinc nitrates deposited via incipient wetness impregnation; (4) AIM-alumina impregned with microemulsion, sol-gel derived alumina impregnated with microemulsion via controlled evaporation.

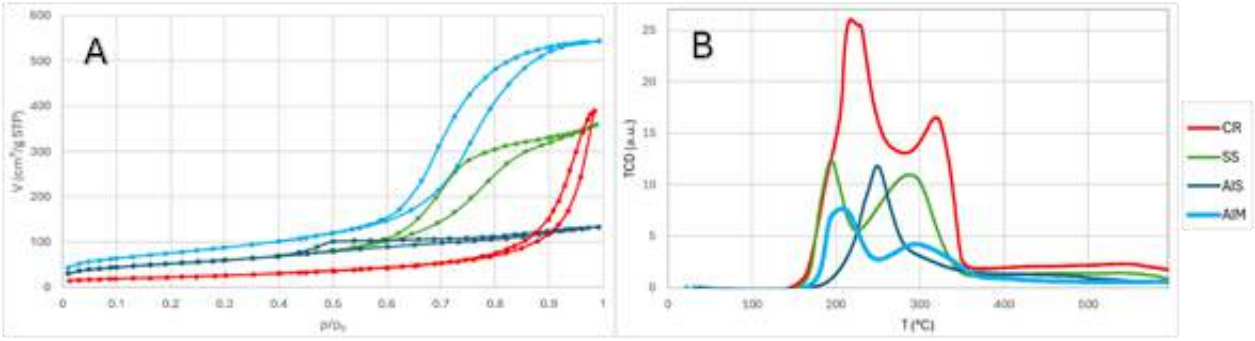

Figure 1. (A) Nitrogen physisorption of the catalysts and (B) TPR.

The SS catalyst demonstrates superior textural properties including high surface area, controlled porosity and enhanced reducibility at lower temperatures relative to the reference catalyst, as illustrated in Figure 1, positioning it as a promising candidate for methanol synthesis.

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FROM SHAPE TO STRENGTH: HOW A SEMI-SPHERICAL DIE TRANSFORMS AA2024-O MICROSTRUCTURE SHEETS THROUGH SEVERE PLASTIC DEFORMATION

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In repetitive corrugation and straightening (RCS), die geometry plays a fundamental role in controlling the deformation conditions imposed on the processed sheet and, consequently, the resulting mechanical response of the material [1, 2, 3]. Alongside characterizing the effects of die type and profile, particular emphasis must be placed on die design to predict and manage stress concentrations and the spatial distribution of equivalent plastic strain [1]. With this objective, a semi-spherical die geometry design was developed and evaluated for the RCS processing of AA2024-O aluminum alloy sheets. Finite element simulations were conducted to examine the distributions of shear stress and equivalent plastic strain in sheets of approximately 1 mm thickness. A processing rate of 0.5 mm/min was applied throughout all simulations. The semi-spherical geometry yielded a uniform equivalent plastic strain distribution, free from strongly concentrated shear regions, suggesting that it may sustain a greater number of processing cycles before the onset of critical localized damage. Following RCS processing, the sheets were characterized by X-ray diffraction and mechanical testing comprising tensile stress–strain experiments and Vickers micro-hardness measurements, following methods well established for RCS-processed aluminum alloys. The semi-spherical die produced enhances the mechanical strength; the yield strength increased 59.5% after the first RCS pass and marginally increases for subsecuent pases. In contrast, the maximum strain dropped 39.1% compared to the as-received material.

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DEVELOPMENT OF LITHIUM NICKELATE ($LiNiO_2$) AS A CATALYST-SORBENT FOR EFFICIENT H_2 PRODUCTION VIA WATER GAS SHIFT REACTION

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In the global context of renewable energies, hydrogen (H_2) production has become a critical area of focus, due to the increase in pollution and greenhouse gas emissions associated with the consumption of fossil fuels.[1] Within this context, the Water-Gas Shift (WGS) process is a chemical reaction used to produce H_2 by converting CO and H_2O into CO_2 and H_2.[2] This reaction typically requires a catalyst, and different ceramic materials have demonstrated significant activity in this role. Ceramic materials containing transition metals like nickel in their structure have been used for H_2 production. In fact, $LiNiO_2$ has been used for CO and CO_2 capture and subsequently as a bifunctional material.[3] In the present work, $LiNiO_2$ was synthesized by ~~a~~ precipitation reaction employing lithium hydroxide (LiOH) and nickel nitrate ($Ni(NO_3)_2$) as precursors.[4] The procedure consisted of mixing the reactants in an aqueous solution and heating until water evaporation. The resultant powder was heat treated at 700 °C for 5 hours, applying a thermal ramp of 10 °C/min under an air atmosphere. The product was characterized using the powder X-ray diffraction (XRD). Its analyses showed the obtention of the pristine phase. Then, through dynamic and isothermal thermogravimetric analyses, it was possible to determine that this nickelate has a high efficiency for capturing CO under CO and equimolar CO-O_2 atmospheres. Following these studies, $LiNiO_2$ catalytic activity was evaluated, using a catalytic reactor coupled to gas chromatography. These experiments also involved dynamic and isothermal conditions, using CO and H_2O flows while varying H_2O vapor molar excesses. The results indicated that optimal operating temperature is 500 °C with a H_2O:CO molar ratio of 4.5, with efficiencies of around 90 %. In addition, although the chromatograms show CO_2 as a byproduct, isothermal solid products were analyzed by XRD, confirming the presence of lithium carbonate (Li_2CO_3). Thus, lithium nickelate captures a fraction of CO_2 through the water gas shift reaction process.

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Design and Production of a Triply Minimal Surface based cellular material by lost polymer casting

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Triply periodic minimal surfaces (TPMS) are mathematically defined surfaces that present zero mean curvature everywhere and repeat periodically along three Cartesian axes. They are similar to smooth and continuous surfaces in nature and are promising for a wide range of technical applications. TPMS show high specific energy absorption; possible applications are thermal management, acoustic absorption, impact absorption and battery electrodes.
Manufacturing methods for metallic TPMS include laser powder bed fusion (LPDF), metal binder jetting and casting. Lost Polymer Casting (LPC) is an economical variation of the traditional lost-wax casting. Instead of creating a prototype from wax, Additive Manufacturing (AM) is used to print a polymeric TPMS sacrificial pattern to create complex geometries such as cylinders with intricate patterns.
The present research involves 3D modelling of a gyroid cylinder by mathematic software and mesh refinement for correct printing. A sacrificial nylon prototype is produced using LPBF. This model is molded by cristobalite. After calcinating the polymer, the molten alloy is poured into the mold to create a TPMS cylinder. Prototypes are characterized by X-ray microtomography and compression tests.

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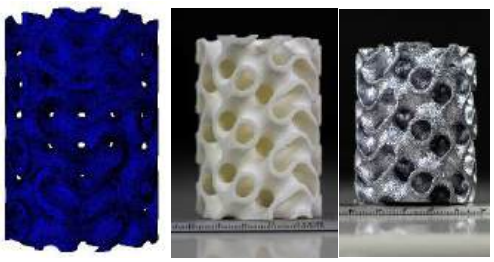

Magnetic and electrical properties of trirutile-structured Fe, CO, and Ni oxides, MTa_2O_6

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Solid-state materials with a trirutile-type structure (AB_2O_6) constitute a family of crystal structures derived from the rutile structure (AO_2), in which the structural periodicity along the c crystallographic axis is tripled relative to the rutile unit cell. In this configuration, the ordering of different cations within a rutile-type structure breaks the periodicity of the rutile structure, giving rise to the formation of a 1 × 1 × 3 superlattice.

In trirutile-based compounds whose general chemical formula is typically written as AB_2O_6, the A sites are occupied by divalent or trivalent cations such as Mg^{2+}, Ni^{2+}, Cu^{2+}, or Fe^{3+}, and the B sites by cations such as Sn^{4+}, Nb^{5+}, Sb^{5+}, Ta^{5+}, or W^{6+}.They exhibit interesting physical properties, such as low-dimensional magnetic ordering, microwave dielectric behavior, magnetoelastic coupling, magnetic properties, and optical properties, among others. Furthermore, they are potential candidates for possible catalytic applications, depending on the cations involved.

We investigated the magnetic and electrical transport properties of $FeTa_2O_6$, $CoTa_2O_6$, and $NiTa_2O_6$ in the 2–300 K temperature range. We synthesized these materials by solid-state reaction and refined their crystal structures by the Rietveld method. These oxides are known as trirutile because they resemble three simple rutile $BO_2AO_2BO_2$ layers stacked along the c-axis. In this system, the ideal cation sequence is BAB, but structural disorder often occurs, making these materials magnetically and electrically interesting. These materials are attractive as photocatalysts because, although the optical gap of the tantalum-based oxides is about 4.1 eV, it can be modulated by the 3d metals incorporated into the crystal cell.

The electrical behavior exhibited by these MTa_2O_6 (M = Fe, Co, Ni) trirutiles is that of a semiconductor in the low-temperature (25–300 K) regime, and magnetically they show an antiferromagnetic behavior, which fits a Curie-Weiss law, with values of Θ_W of about 13 K (Fe^{2+}), 15 K (Co^{2+}), and 22 K (Ni^{2+}). In the 100–300 K range, they show paramagnetic behavior, with magnetic moments of 5.6 Bohr magnetons (μ_B) (Fe^{2+}), 5.24 μ_B (Co^{2+}), and 3.38 μ_B (Ni^{2+}). We also spectroscopically characterized these MTa_2O_6 materials by diffuse reflectance in the UV-vis range and determined their optical gap. These values make these materials attractive as photocatalysts in the visible range of the electromagnetic spectrum.

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Hydrogenolysis of Lignin Model Compounds and Native Lignin over Co-N-C Catalyst

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In this work, cobalt-based M-N-C catalysts were synthesized and evaluated for the transfer hydrogenolysis of lignin-derived compounds. The Co-800 material, consisting of cobalt nanoparticles (CoNPs) together with subnanometric Co(II) species dispersed within a nitrogen-doped carbon framework, exhibited excellent activity and selectivity toward the cleavage of C-O bonds in oxidized β-O-4 lignin model compounds using formic acid as a hydrogen source. To investigate the role of the cobalt nanoparticles, Co-800 was subjected to acid leaching, producing the Co-800-AT catalyst. Despite the removal of CoNPs, Co-800-AT preserved considerable catalytic performance, suggesting that atomically dispersed cobalt species play a key role in the reaction. Both catalysts showed efficient operation under relatively mild reaction conditions, while Co-800 maintained high conversion levels and good recyclability through successive reaction cycles. Overall, these results highlight the potential of cobalt-based M-N-C materials as durable and sustainable catalysts for lignin valorization and depolymerization processes [1- 4].

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Electrical conductivity in Nb^{5+}-doped $Y_2Ti_2O_7$ pyrochlore: the effect of possible interstitial oxygen migration

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Solid electrolytes are important in developing electrochemical energy storage, conversion, and generation devices. Yttria-stabilized zirconia (YSZ) is the most representative solid electrolyte for O^{2-} ionic conduction [1], and several studies have improved YSZ structural and chemical properties to obtain new solid electrolytes such as rare-earth-doped ceria or complex perovskites. This work presents the electrical transport behavior of $Y_2Ti_2O_7$ with a pyrochlore structure (PS). The PS is related to the YSZ fluorite structure [2], [3], but it has 12.5% more oxygen vacancies than the regular fluorite structure. Additionally, $Y_2Ti_2O_7$ was doped with a donor aliovalent ion (Nb^{5+}). Rietveld refinements of powder XRD patterns showed that doping did not modify the PS. Additionally, a linear relationship was found between the lattice parameter and dopant content, implying a solid-solution system in the $0.0 > x > 0.2$ range in the $Y_2Ti_{2-x}Nb_xO_{7+x/2}$ system. The best electrical conductivity was measured in a nitrogen atmosphere, and under this condition, donor doping enhanced electrical conductivity (Figure 1), indicating that ionic conduction could occur via interstitial migration; a similar effect has been reported for other donor-doped PS compounds ($Gd_2Zr_2O_7$).

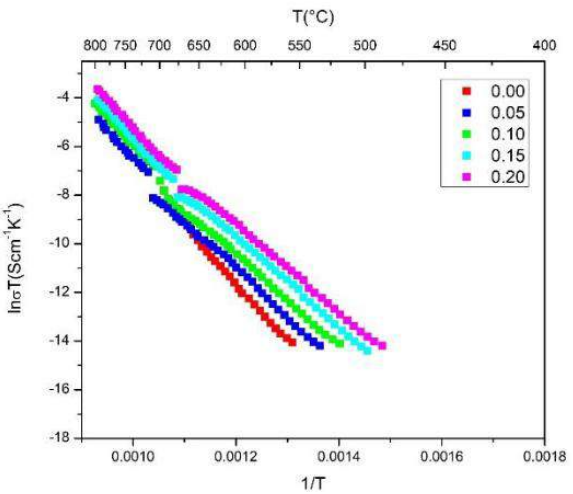

Figure 1. Arrhenius-type plot for electrical conductivity of the $Y_2Ti_{2-x}Nb_xO_{7+x/2}$ system. The electrical conductivity increased with donor dopant content.

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Effect of fabrication route and heat treatment on the microstructure of a TiNbZrTaMoHf refractory high-entropy alloy for biomedical applications

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Refractory high-entropy alloys (RHEAs) represent promising materials for engineering and biomedical applications. Several such alloys have been investigated to examine the correlation between their microstructure and mechanical properties [1]. In this context, understanding the effect of different fabrication routes and heat-treatment conditions is essential for clarifying potential amorphous phase formation, elemental segregation, and phase stability [2]. This work investigated the microstructure and mechanical properties of a TiNbZrTaMoHf RHEA prepared from the liquid state and heat-treated. The composition was previously selected using thermodynamic calculations and artificial intelligence techniques [3]. Phase constitution and chemical distribution were examined by X-ray diffraction with Rietveld refinement and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy. Besides, Vickers microhardness was measured to assess the mechanical response. In general, the alloy is composed of BCC1-BCC2 phases and exhibits a dendritic microstructure. Regarding the heat-treated condition, the process promoted HCP-phase formation and partially destroyed the dendritic microstructure, yielding a predominantly BCC+HCP dual phase alloy and a slight increase in the microhardness values. These results demonstrate that fabrication route and thermal treatment significantly modify the phase formation and the microstructure. Such differences may influence the mechanical, corrosion, tribological, and ion-release behavior, emphasizing the need to select the processing conditions according to the intended application.

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ELECTRODE MATERIALS FOR K-ION BATTERIES

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To support the global transition toward renewable energy, the development of efficient electrochemical energy storage systems is essential. While lithium-ion batteries (LIBs) dominate the market, their large-scale application is hindered by lithium's scarcity (0.0017 wt % in the Earth crust), high extraction costs, and uneven distribution. K-ion batteries (KIBs) offer a compelling alternative due to potassium abundance (1.5 wt% in the Earth crust) and a standard reduction potential comparable to lithium (Li^+/Li = -3.04 V, K^+/K = -2.93 V *vs.* SHE) [1]. However, the larger ionic radius of K^+ induces severe volume expansion and rapid degradation in traditional electrodes, necessitating the design of novel electrode materials.

In this context, this communication explores metal chalcogenides, specifically tin sulfide (SnS) and chalcopyrite ($CuFeS_2$), as highly promising KIB electrodes [2]. These materials operate via a conversion-based mechanism that delivers exceptionally high theoretical capacities, while their relatively weak metal-sulfur bonds provide more favorable reaction kinetics than metal oxides, commonly used in LIBs [3].

In this work, both sulfides were synthesized through a rapid and highly efficient microwave-assisted hydrothermal method and structurally characterized using x-ray and neutron diffraction as well as high-resolution transmission electron microscopy (HRTEM). Finally, their electrochemical performance was optimized. We will discuss the impact of key variables such as synthesis time, the ratio of active material to conductive additive and potential window, amongst others, on its electrochemical performance.

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THERMO-CALC ANALYSIS OF LOW-MELTING MULTIPRINCIPAL ELEMENT ALLOYS

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Low-melting multiprincipal element alloys (LMMEAs) have recently attracted attention from the scientific community because the formation of single phases has proven very challenging. In this work, Al-Zn-Cu-Ag-X (X = In and Sn) have been investigated with different amounts of the low-melting-point metal to produce LMMEAs for possible processing into metallic foams. Thermo-Calc analysis was carried out to simulate the one-axis phase diagram in order to obtain the phase transformations of a particular alloy composition as a function of temperature. The results showed that for the quaternary, only three phases crystallized in equilibrium at room temperature; however, when adding the fifth element, another phase crystallizes, producing a more complicated structure. On the other hand, it was possible to theoretically obtain alloys of the abovementioned compositions with low melting temperatures (<600°C) for the possible production of the first reported low-melting multiprincipal element metallic foams.

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CO_2 Fixation and Olefin Oxidation with Cobalt-Guanidine-Benzimidazole Systems and a Supported Ionic Liquid Phase

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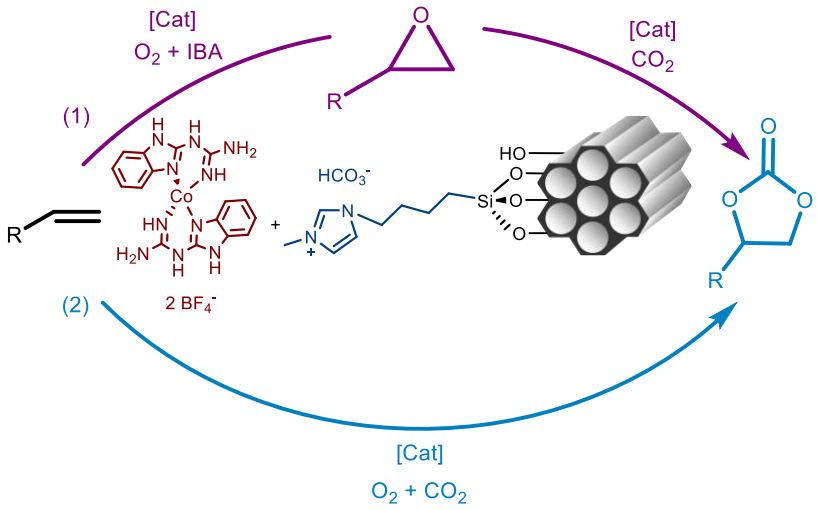
The combination of benzimidazole and guanidine moieties within a single ligand framework has emerged as a powerful design strategy in bioinspired coordination chemistry, drawing from the complementary electronic and hydrogen-bonding properties of both functional groups. Benzimidazole offers strong nitrogen coordination akin to histidine residues in metalloenzymes, while guanidine introduces a basic site capable of proton transfer and secondary sphere interactions, reminiscent of arginine in enzymatic active sites. When coordinated to cobalt, these hybrid ligands provide a multifaceted environment that enhances the metal center's ability to activate small molecules. This has proven especially advantageous in the catalytic conversion of carbon dioxide to value-added products and in promoting selective oxidation reactions, where the cooperative action of both ligand components facilitates substrate binding, activation, and stabilization of reactive intermediates, thus mimicking key features of natural catalytic systems. In this study, a cobalt(II)-based SILP catalyst functionalized with imidazolium hydrogen carbonate ([BMIm][HCO_3]) was synthesized and evaluated in oxidative carbonylation reactions. The discrete complex [Co(GBImz)$_2$][BF_4]$_2$, bearing guanidine-benzimidazole ligands, showed limited CO_2 fixation capacity but exhibited notable potential in olefin oxidation, suggesting its suitability for one-pot oxidative transformations.



Microstructural Evolution and Recoverable Inelastic Deformation in a Mg- based alloy after Solution Heat Treatment.

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Abstract

Currently, the most common materials used for temporary orthopedic implants are not compatible with natural bone, which impairs bone healing. To address these issues, magnesium-based alloys are very promising options due to their biocompatibility and mechanical properties, which closely resemble those of natural bone [1].However, their mechanical response may involve reversible inelastic deformation, which is often overlooked in conventional evaluations of elastic properties[2-3]. Ignoring this contribution can lead to an inaccurate determination of the apparent stiffness of magnesium-based biomaterials and, consequently, affect the assessment of load transfer between the implant and the surrounding bone [3]. In this study, the macroscopic behavior of reversible nonlinear deformation of a Mg–Zn–Ag alloy was investigated as a function of the duration of solid-solution heat treatment [4]. Uniaxial compression-strain tests revealed a well-defined nonlinear transition regime, characterized by a rounded “knee” in the stress-strain response and associated with Stage II deformation, under all investigated conditions (SS24h, SS48h, and SS120h). The magnitude and prominence of this nonlinear response increased progressively as the solution treatment time increased. This evolution is attributed to progressive microstructural homogenization, partial dissolution, and redistribution of secondary phases, as well as to a higher concentration of solute atoms within the α-matrix.

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ZnCdS PHOTOCATALYSTS FOR ANTIBIOTICS DEGRADATION

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Abstract

The growing presence of emerging contaminants in aquatic ecosystems, particularly antibiotics, poses serious threats to human health because they can drive antimicrobial resistance [1]. Consequently, it is necessary to develop advanced, sustainable, and low-cost technologies, such as heterogeneous photocatalysis, to efficiently degrade antibiotics in water under visible-light irradiation [2]. Among the studied photocatalysts, CdS stands out for its good stability and adjustable bandgap, which offers great potential for antibiotic degradation and hydrogen production [3]. In this study, a $Zn_{0.5}Cd_{0.5}S$ solid solution was prepared using the hydrothermal method with $Cd(NO_3)_2{\cdot}4H_2O$, $Zn(CH_3COO)_2{\cdot}2H_2O$, and $Na_2S{\cdot}9H_2O$ as precursors. The precursors mixture was stirred for 30 min, then transferred to a stainless-steel-lined reactor and heated to 200 °C for 20 hours. X-ray diffraction results showed that the photocatalysts exhibit the wurtzite phase. Diffraction reflections shifted slightly to larger angles as Zn was introduced into the CdS structure, demonstrating the formation of a solid solution. The bandgap value of CdS was determined to be 2.40 eV, while that of $Zn_{0.5}Cd_{0.5}S$ was 2.55 eV. The photocatalytic performance of the materials was evaluated by the degradation of tetracycline (TC) under visible radiation using a solar radiation simulator. For the test, a TC solution (50 mL, 15 mg/L) and 20 mg of photocatalyst were stirred in total darkness for 30 min; subsequently, solar simulator irradiation started. Aliquots were taken every 10 min over a 60 min period, and the concentration was measured using a UV-Vis spectrophotometer to determine the degradation efficiency of the materials. After 60 minutes of exposure, TC removal was 42% for CdS and 73% for ZnCdS. The decrease in pH of the TC solution from 6.2 to 4.2 increased degradation to 83 %. Compared with CdS, Zn significantly enhances the photocatalytic performance of CdS due to its structural stability.

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HFCVD-GROWN MoO_3 THIN FILMS FOR CONDUCTOMETRIC GAS-SENSING APPLICATIONS

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Molybdenum oxide (MoO_3) is a semiconductor with structural and electronic properties of interest for the development of conductometric gas sensors [1]. In this work, nanostructured MoO_x thin films were synthesized by hot filament chemical vapor deposition (HFCVD) [2], a technique that remains scarcely explored for the preparation of this material. The films were deposited on silicon substrates using a molybdenum filament and subsequently annealed at 300, 400, and 500 °C to evaluate the effect of thermal treatment on their properties. X-ray diffraction and Raman spectroscopy revealed an evolution from a poorly ordered as-deposited material toward a crystalline structure consistent with orthorhombic α-MoO_3, particularly after annealing at 500 °C. Electron microscopy showed progressive morphological changes and the formation of more clearly defined nanostructures with increasing annealing temperature. XPS analysis confirmed Mo^{6+} as the predominant oxidation state, together with a minor contribution of Mo^{5+} species. In addition, the films exhibited a photoelectrical response under UV irradiation, with the sample annealed at 500 °C showing lower electrical resistance and a more stable and reproducible response. These results demonstrate the feasibility of HFCVD for the synthesis of nanostructured MoO_3 thin films and their potential use as active layers in gas-sensing devices.

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CHARACTERIZATION OF Zr-Hf-Nb BASED HIGH-ENTROPY ALLOYS DESIGNED BY ARTIFICIAL INTELLIGENCE

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High-entropy alloys have attracted considerable interest in various research areas due to their excellent mechanical, thermal, and corrosion properties, which stem from the effects of high configurational entropy, including large lattice distortion, slow diffusion, and the cocktail effect [1]. The Zr-Hf-Nb ternary system has been of interest because it exhibits superplasticity during compression testing, reaching up to 80% deformation without fracture. However, it is unknown how adding new elements and increasing alloy entropy would affect the material's superplasticity. In this work, a design-assisted approach was used with the NSGA-II algorithm, which is a method inspired by natural selection and combines evolutionary algorithms and artificial neural networks [2] to select two compositions within the Zr-Hf-Nb-V-Ti-Mo senary system: one equiatomic ($Zr_{16.65}Hf_{16.68}Nb_{16.65}V_{16.66}Mo_{16.68}Ti_{16.67}$ at%) and another non-equiatomic with a higher Nb content ($Zr_{7.79}Hf_{18.41}Nb_{42.72}V_{20.21}$ $Mo_{3.52}Ti_{7.35}$ at%). The alloys were synthesized by electric arc casting, starting from a Mo-Zr master alloy to facilitate Mo dissolution, and cylindrical specimens (6mm diameter) were subsequently obtained by suction casting. Structural characterization included XRD, optical and electron microscopy (SEM-EDS, TEM-EDS, and EBSD), while mechanical properties were evaluated using compression and Vickers microhardness tests. Phase diagrams obtained with Thermo-Calc predict a single BCC phase for both compositions, corroborated by XRD diffractograms and EBSD analysis using AZtecCrystal software. Compression test results indicate high plasticity with deformations of up to 80%, maintaining the superplasticity of the base material as defined by the algorithm used. Similarly, microhardness values show homogeneous behavior throughout the material, exhibiting high hardness with significant deformation capacity.

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EFFECT OF CALCIUM SUBSTITUTION AT THE B SITES OF THE BCZT COMPOUND ON ITS STRUCTURE, PIEZO-DIELECTRIC PROPERTIES AND ELECTRONIC STRUCTURE

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The current work presents experimental and theoretical evidence of how the migration of Ca^{2+} ions from the A-site to the B-site (occupied by Ti and Zr) within the perovskite-type structure of the $Ba_{1-x}Ca_xTi_{0.9}Zr_{0.1}O_3$ (BCTZ) compound affects its crystal structure, dielectric and piezoelectric properties, and electronic structure. The BCTZ compound was prepared via the Pechini method. The pressed pellets were sintered in air at 1400 °C for 4 h. In the first stage, Raman spectroscopy reveals a signal centered at 800 cm^{-1} (analyzed using the Fityk program), associated with the migration of Ca^{2+} ions from the A-site to the B-site in octahedral (O_h) coordination [1]. Subsequently, changes in the octahedral volume are monitored by refining X-ray diffraction patterns (using the FullProf Suite software) to obtain a crystallographic information file (CIF) containing structural data—specifically regarding the octahedron—which is visualized using the VESTA program [2]. In the second stage, dielectric curves are interpreted to demonstrate relaxor behavior attributed to chemical substitution at the B-sites by the Ca^{2+} acceptor ion. In the third stage, a multiplet calculation (using CTM4XAS software) [3] is proposed to reproduce the spectral profile characteristics of electron energy loss spectra (EELS) at the Ca $L_{2,3}$-edge. The modeling considers Ca^{2+} in an octahedral (O_h) coordination with a crystal field energy of 1.2 eV [4].

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WEAR RESISTANCE, CORROSION AND BIOACTIVITY OF Al_2O_3–TiO_2 AND Al_2O_3–TiO_2/HA COATINGS DEPOSITED BY APS ON 316L STAINLESS STEEL

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This study explores the tribological and electrochemical behavior of Al_2O_3–TiO_2 and Al_2O_3–TiO_2/hydroxyapatite (HA) coatings deposited on 316L stainless steel using Atmospheric Plasma Spraying (APS) for biomedical applications. Although 316L stainless steel is commonly used in orthopedic implants due to its strength and reliability, it remains prone to corrosion and ion release in physiological environments and does not naturally promote bone integration. In this context, surface modification through APS offers a promising way to improve both; durability and biological performance. The coatings were analyzed using Scanning Electron Microscopy and X-ray Diffraction to understand their structure and phase composition. Their mechanical properties were evaluated through microhardness and adhesion tests, while corrosion experiments in simulated body fluid were conducted to assess their chemical stability under body simulated conditions. The capability of coatings to grow bone like compounds was examined through immersion tests, followed by surface analysis. Results show that coatings significantly improved both; corrosion and wear resistance. In particular, the addition of HA enhances apatite formation, indicating bone-bonding potential. Overall, these coatings offer an effective means of transforming a commonly used biomedical material into a more durable, biologically and surface activated option, with potential benefits for implant longevity.

Keywords: Atmospheric Plasma Spraying, Bioactivity, Bio-ceramic Coatings

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Mössbauer spectroscopy: A high-resolution nuclear technique for materials characterization

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This presentation provides an introductory overview of Mössbauer spectroscopy and its applications in materials science. It details the three primary hyperfine parameters derived from the potential distribution, $V(r)$, around an iron nucleus: isomer shift (δ), quadrupole splitting(Δ) , and the hyperfine magnetic field (H_{hyp}) , emphasizing their fundamental relationship to the characterization of the local electronic environment. Additionally, the inherent advantages and limitations of this spectroscopic technique are evaluated. Finally, a discussion on the interpretation of these hyperfine parameters is presented, utilizing various practical examples to illustrate their descriptive capabilities across a diverse range of material systems.

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Structural and electronic characterization of the $BiFe_2MO_7$ (M = Nb, Sb and Ta) pyrochlores

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Polycristalline samples of nanostructurted pyrochlores were synthesized by the molten salts method in 5 minutes at 950 °C. The structural characterization was performed by X-Ray diffraction (XRD) and scanning electron microscopy (SEM) while the electronic characterizaton was done througth Mössbauer (MS), diffuse reflectance (DRS) and X-ray photoelectron (XPS) spectroscopies. XRD confirms the pure phase $BiFe_2MSbO_7$ pyrochlores, while SEM evidence the nanostructure nature of the samples. MS shows the iron cation distribution in both crystallographic sites while XPS shows a distortion in the Bi core-level region as a consequence of Nb, Sb and Ta cation sustitution, correleting well with MS results. Finally, the DRS results lets to stimate the optical band gap, suggesting this materials as promising active semiconductors under UV-visible irradiation.

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Ga-In-Bi-Sn-Ag-BASED HIGH-ENTROPY: LOW-MELTING-POINT ALLOYS FOR ELECTRONIC SOLDERING

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Environmental and health concerns associated with conventional Sn-Pb solders have accelerated the development of lead-free alternatives. In this context, low-melting-point high-entropy alloys (LMP-HEAs) have emerged as promising candidates for advanced soldering applications. In this work, we investigate the Ga-In-Bi-Sn-Ag system as a candidate LMP-HEA using a combined theoretical and experimental approach to identify compositions with low melting points, good mechanical properties, high wettability, and enhanced corrosion resistance. Thermodynamic simulations using Thermo-Calc software led to the selection of four alloy compositions, minimizing experimental iterations. Experimental results showed strong agreement with predictions from the thermodynamic calculations, validating the simulations for phase formation and thermal behavior. Structural and thermal characterizations revealed complex, multiphase microstructures predominantly composed of BiIn, β-Sn, and In-Sn phases, along with minor amounts of additional elemental or intermetallic phases. Differential scanning calorimetry indicated melting transitions below 90 °C for all compositions except the equiatomic alloy, which remained partially solid up to 240 °C. Among the studied compositions, $Ga_5In_{30}Bi_{30}Sn_{30}Ag_5$ stands out as a promising candidate because of its refined, homogeneous microstructure, low melting point (84°C), highest compressive strength (57.4 MPa), and compressive plastic behavior (>100%). Additionally, wettability tests on PDMS substrates demonstrated favorable spreading behavior, with a contact angle of 52° at 180 °C for this alloy. Finally, corrosion tests in saline media revealed high corrosion resistance for all alloys, outperforming commercial lead-free solders.

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Hydrogen production using the $Na(Co_{1-x}Ni_x)O_2$ solid solution as sorbent-catalyst in reforming reactions

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The energy demand increments are leading to a larger presence of renewable energy sources worldwide. However, due to its intermittency caused by climatic and geographical factors, there is a push to find solutions to this problem.[1] A viable alternative to this problem is the use of hydrogen (H_2) as an energy carrier vector, due to its high energy density and the fact that its application does not release pollutants, unlike fossil fuels.[2] However, its large-scale implementation still faces significant challenges, primarily related to production efficiency, risks posed by its high flammability, and the lack of suitable materials for safe storage.[3]
In this context, the production of H_2 using alkaline ceramic materials is attracting interest. Furthermore, the development of solid solutions offers tunable physicochemical properties, allowing to the modification of catalytic activity, oxygen mobility and —surface reactivity—all [4] of which contribute to improve H_2 production. These characteristics make alkaline ceramic materials suitable for application in high-temperature reactions such as, wet reforming or water-gas shift (WGS).
In this study, a solid solution based on nickel-containing sodium cobaltate ($NaCo_{1-x}Ni_xO_2$) was synthesized, and its performance was evaluated as a bifunctional material for carbon dioxide (CO_2) capture and H_2 production. Different compositions of this solid solution were characterized using various techniques to confirm structural changes and morphological characteristics. Then, dynamic and isothermal thermogravimetric analyses were also performed in CO_2 and carbon monoxide (CO) atmospheres to evaluate their capture capacity. Furthermore, catalytic performance was evaluated under dynamic wet reforming and WGS conditions, for H_2 production. Results show that this $NaCo_{1-x}Ni_xO_2$ solid solution does exhibits the proposed bifunctional characteristics: CO_2 sorbent and H_2 production catalyst.

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DEVELOPMENT OF CdS PHOTOCATALYSTS FOR ANTIBIOTIC DEGRADATION APPLICATIONS

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Abstract

The presence of antibiotics in water bodies represents an emerging environmental problem due to their high persistence and contribution to antimicrobial resistance [1]. In this context, heterogeneous photocatalysis using visible-light-activated semiconductors has attracted significant interest as a strategy for degrading recalcitrant organic pollutants [2-3]. This study reports the hydro/solvothermal synthesis of the semiconductor cadmium sulfide (CdS) in a water-ethylenediamine (1:3) mixture and evaluates the influence of the sulfur precursor, synthesis time, temperature, and the presence of the surfactant polyvinylpyrrolidone (PVP) on the morphology and catalytic properties of the samples. A two-stage study was developed; first, the effect of sulfur sources (thiourea and L-cysteine) on the formation of CdS nanostructures was evaluated. Subsequently, synthesis parameters such as temperature, reaction time, and PVP use were investigated to control crystal growth and promote structures with higher surface area. The materials were synthesized at 150 and 200 °C for 8 and 12 hours and characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-Vis spectroscopy, aiming to correlate composition, morphology, and optical properties with photocatalytic performance. The results showed that morphology depends primarily on the sulfur precursor, followed by temperature and synthesis time, whereas PVP showed no influence. Samples obtained using L-cysteine exhibited nanowire microstructures, while those synthesized with thiourea displayed flower-like structures. Furthermore, samples synthesized using L-cysteine and thiourea exhibited a hexagonal CdS phase and bandgap energy that decreased as temperature increased. Photocatalytic activity, evaluated via tetracycline degradation under simulated solar light irradiation (1000 W), showed degradation rates between 80% and 88%; specifically, samples synthesized with L-cysteine (12 h) and thiourea (8 h) at 150°C without PVP achieved degradation levels of 88% and 87%, respectively, after 1 hour of irradiation.

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Influence of composition and different atmospheres in the electrical conductivity of Wadsley-Roth phases based on Nb/W oxides.

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Wadsley–Roth (WR) phases have been studied as anode materials for Li-ion batteries due to their unique structural properties. Their crystal structure contains channels that enable ion storage and fast ion transport throughout the lattice, allowing the intercalation of large amounts of lithium (up to 400 mAh g^{-1}) at an operating voltage of approximately 1.6 V, values comparable to those of the $Li_4Ti_5O_{12}$ anode. [1,2]

WR phases are based on transition metals such as Nb, Ti, W, and V, and exhibit two main structural types (Figure 1): (a) columns of pentagonal bipyramids $\{M\}X_7$ sharing each equatorial edge with $\{M\}X_6$ octahedra, and (b) a distorted ReO_3-type structure. These structures contain cavities that facilitate rapid ion transport. The stability of these phases depends on the number and nature of the shared vertices between neighboring metal–oxygen octahedra. [2]

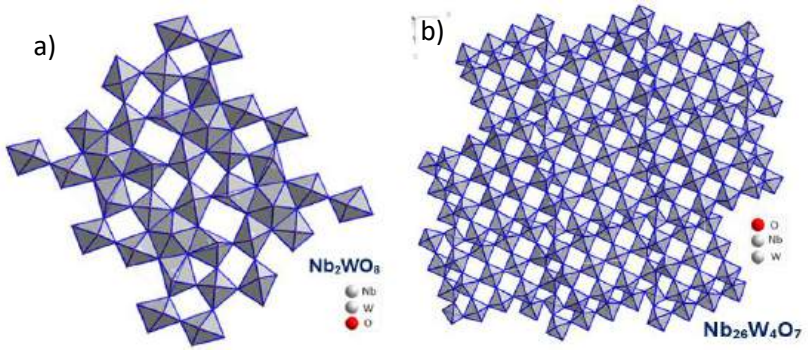


Figure 1 Different types of structure in Wadsley-Roth phases a) pentagonal bipyramids and b) ReO_3 distorted.

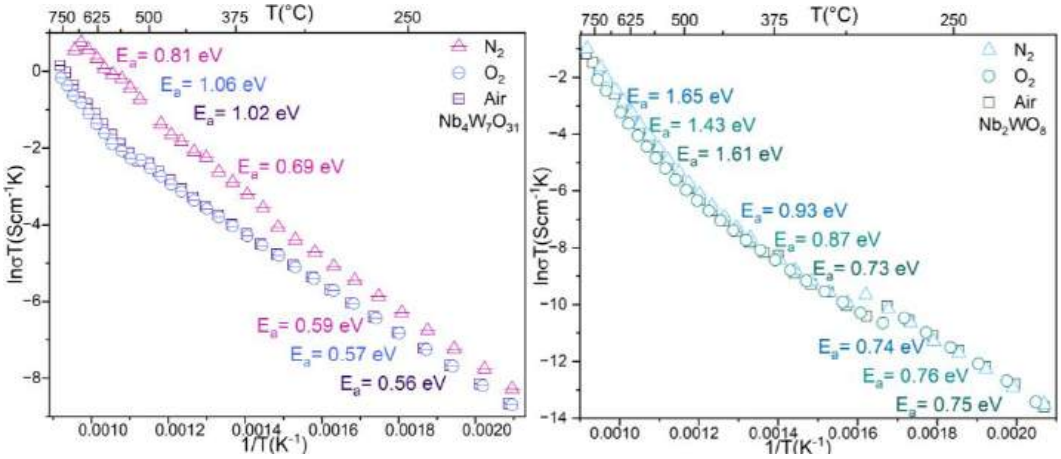
In this work, the influence of Nb/W ratio over the conductivity using three different atmospheres (N_2, O_2 and air) was investigated. The compounds $Nb_4W_7O_{31}$ (W/Nb ratio= 0.64) and Nb_2WO_8 (W/Nb ratio= 0.33) were synthesized by conventional solid-state reaction metod at 1100 °C for 96 h, and sintered at 1150 °C for 12 h, obtaining compounds with pentagonal structure (type a in Figure 1). Both compounds were studied in the same conditions for each atmosphere:

The Arrhenius type plot (Plot 1) show that $Nb_4W_7O_{31}$ exhibits oxygen ion mobility from 500 to 800 °C and electronic mobility seems to occur from 200 to 500 °C in O_2 and air atmospheres. Incontrast, under N_2 atmosphere a redox process is observed over 690 °C and electronic mobility occur at the same temperature (200 to 500 °C) but with a higher activation energy.

On the other hand, Nb_2WO_8 exhibits the same behavior in the three atmospheres (N_2, O_2 and air), with similar activation energies in N_2 and air. Under an O_2 at temperatures above 460 °C present

the lowest activation energy for oxygen ion mobility in this compound and no evidence of redox behavior was observed.

$Nb_4W_7O_{31}$ exhibits the highest conductivity, increasing by approximately two orders of magnitude under reducing conditions. Furthermore, its activation energy is lower than Nb_2WO_8. In Nb_2WO_8 In contrast, oxygen ion mobility in Nb_2WO_8 begins at 460 °C, whereas in $Nb_4W_7O_{31}$ it happens until 500 °C.



Plot 1 Arrhenius-type graphs for $Nb_4W_7O_{31}$ and Nb_2WO_8 in different atmospheres.

Overall, doubling the tungsten ratio in the compound enhanced the electrical conductivity of the material due to the partial reduction of tungsten at the surface, which increases the metallic character of the bonding and promotes electron transport throughout the material. Both compounds exhibit mixed ionic-electronic conduction at different temperatures.

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SYNTHESIS OF LTA ZEOLITE MEMBRANE ON MODIFIED SURFACE OF ZrO_2: EFFECT OF COUPLING AGENT

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The development of zeolite-based membrane has increased in the last decades due to diversity of applications in environmental, separation processes, and biomedicine [1,2]. This is because of their biocompatibility, biological stability and shape and size selectivity. To achieve a uniform growth of zeolitic phase on the support, parameters such as the support, its modification, the synthesis method, and zeolite topology, are crucial. For these reasons, in the present work the formation of LTA zeolite membrane on zirconium oxide was studied. The synthesis was carried out by second growth method. The surface support was submitted to chemical modification using three different coupling agents: 3-mercaptopropyl trimethoxysilane (MPS), trimethoxysilyl propylmethacrylate (TMPM) and polyvinyl sulphonic acid (PVSA). Subsequently, the supports were rubbed with LTA zeolite crystals seeds. Then the support was submitted to hydrothermal treatment using a reaction mixture of molar composition corresponding to LTA zeolite phase. The final products were characterized by XRD, SEM/EDS and FTIR techniques. The findings showed the growth of LTA zeolite on the surface support, it was observed a favorable effect between coupling agent and zirconium oxide support that promoted the formation of the zeolitic membrane. The nature of coupling agent was decisive for the uniformity, thickness and morphology of zeolite membrane, being favored by the support modified by MPS. This zeolite membrane exhibited bioactivity in vitro; therefore it opens up the possibility to conducting further research to determine its potential for biomedical applications.

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Abstract preparation

Gd-doped ZnO nanoparticles: synthesis, structural and optical study, and antimicrobial activity against *Staphylococcus aureus*

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Zinc oxide (ZnO) is a semiconductor exhibiting interesting optical, electrical, piezoelectric, photocatalytic, and antimicrobial properties that are relevant for various nanotechnology applications. However, certain property-related limitations can restrict specific applications; consequently, rare-earth doping has been adopted to enhance ZnO's performance. In this study, Gd-doped ZnO nanoparticles were synthesized via mechanical milling using various synthesis times (1, 3, 9, 30, 90, and 360 minutes). The samples were analyzed using X-ray diffraction (XRD) and ultraviolet-visible spectroscopy (UV-Vis), and their antimicrobial properties against *Staphylococcus aureus* were evaluated using the disk diffusion method. The analyses confirm the incorporation of Gd atoms into the ZnO matrix. Furthermore, the bandgap energy of the samples was determined to be greater than 3.5 eV. It was also observed that the primary activity against the bacterium under study is attributable to the ZnO itself, with Gd showing no significant effect—a result likely due to the generation of reactive Zn^{2+} species.

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FROM MOLECULAR COMPLEXES TO MOF-SUPPORTED CATALYSTS: BUILDING ROBUST CATALYTIC PLATFORMS

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Immobilization of well-defined molecular catalysts on solid supports provides access to hybrid materials that combine the tunability and selectivity of molecular organometallic complexes with the robustness and recyclability of heterogeneous systems. However, preserving the molecular identity and reactivity of the active site remains challenging, while catalyst lifetime and stability are increasingly recognized as key considerations for practical applications.[1] In this context, we have explored Metal–Organic Frameworks (MOFs) as supports for discrete organometallic fragments, exploiting their well-defined porous environments to enhance catalytic properties.

Herein we present Ni, Rh, and Ir complexes supported by semirigid E-phosphine ligands (E = Si, Ge, Sn) and their incorporation into solid supports. These molecular and hybrid systems catalyze hydrosilylation, dehydrogenative silylation, hydroboration, and dehydrogenative borylation of alkenes, with immobilization influencing activity, selectivity, and robustness. As a representative example, grafting [Rh(κ³(P,Si,Si)-PhP(2-$C_6H_4CH_2Si^iPr_2)_2$)] onto NU-1000 through Rh–O–Zr linkages generates a robust hybrid catalyst for styrene dehydrogenative silylation. Compared with its molecular counterpart, the MOF-supported system shows enhanced productivity and selectivity, recyclability over five cycles, and improved aerobic stability. These results demonstrate how interactions between molecular organometallic sites and porous MOF environments can generate robust hybrid catalysts with enhanced reactivity.[2]

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Engineering Robust Plasmonic Nanoparticles with Mesoionic Carbenes: From Polymeric Ligands to Electronic Tuning

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Plasmonic nanoparticles (NPs) have unique optical, catalytic and electronic properties that strongly depend on their size, composition and surface chemistry. *N*-Heterocyclic carbenes (NHCs) have emerged as promising alternatives to conventional thiol-based ligands for the stabilization and functionalization of plasmonic NPs due to their strong carbon–metal bonds and structural tunability [1]. Nevertheless, displacement of surface-bound NHCs under harsh conditions, particularly in the presence of biologically relevant thiols, can still limit the stability and applications of these nanomaterials.

In this talk, we primarily discuss the use of polymerized 1,2,3-triazole-based mesoionic NHCs (*m*NHCs) for the preparation of robust plasmonic NPs. Polymeric *m*NHC–Au(I) complexes were synthesized and subsequently reduced to form water-soluble AuNPs protected by a catenated network of carbene ligands [2]. These materials showed high stability under various conditions. Extending this strategy to silver provided polymeric *m*NHC-stabilized AgNPs with improved stability relative to their monomeric counterparts while maintaining their catalytic activity [3]. Bimetallic polymeric *m*NHC–Au(I)/Ag(I) complexes were also used as precursors to AuAg NPs [4]. Interestingly, variation of the Au-to-Ag ratio within the polymeric precursor controlled the formation of either alloy or Au-core/Ag-shell NPs.

Finally, our recent development of electronically tuned, ester-conjugated 1,2,3-triazole-derived *m*NHCs will be presented. Incorporation of the ester functionality increases the π-acceptor character of the carbene while preserving its σ-donor ability. The resulting changes in metal–carbene bonding considerably enhance the resistance of AgNPs toward thermal, oxidative and thiol-induced degradation and slow the oxidation of highly air-sensitive CuNPs.

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Influence of Homogenization on the Microstructure and Hardness of a Fe–Mn–Al–Si–Cr–C High Entropy Steel under Different Solidification Conditions

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Microstructural control through heat treatment is critical for tailoring the properties of high entropy steels (HES). In this work, the effect of homogenization on the microstructure and hardness of a Fe–Mn–Al–Si–Cr–C high entropy steel was systematically investigated considering two distinctinitial solidification conditions: as-cast and remelted. Homogenization treatments were performed at 1150 °C for 6 h and 12 h in order to evaluate diffusion-driven microstructural changes. The as-cast condition exhibited pronounced chemical segregation, lamellar features associated with solidification, and the presence of complex Mn–Si–Cr-rich precipitates. In contrast, the remelted condition showed a refined microstructure with reduced microsegregation, suggesting differences in heat extraction during solidification. Homogenization led to partial dissolution of secondary phases, redistribution of alloying elements, and coarsening of the remaining precipitates, resulting in a more homogeneous microstructure. The stability and distribution of the ordered FeAl (B2) phase were strongly affected by both homogenization time and initial solidification condition. Microhardness measurements revealed that the as-cast condition exhibited the highest average hardness (~450HV), while homogenization resulted in a decrease to approximately 429 HV after 6 h, followed by a slight increase to ~445 HV at longer holding times (12 h), which is associated with precipitate coarsening. The remelted condition showed intermediate hardness values (~431 HV) with lower dispersion, indicating improved microstructural uniformity. These results demonstrate that homogenization plays a dominant role in controlling microstructural homogeneity and mechanical response, while the initial solidification condition defines the initial distribution of phases and compositional gradients. The combined effect of both factors provides a useful framework for tailoring the properties of high entropy steels through post-solidification processing.

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Refractive index and optical bandgap engineering of RF-sputtered silicon oxynitride thin films from SiO_2 to Si_3N_4

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Silicon oxynitride (SiON) is a key material for integrated photonics because its optical constants lie between those of SiO_2 and Si_3N_4, but reaching the full window with a single, low thermal budget process is still a practical challenge [1]. In this work we show that RF magnetron sputtering of Si_3N_4 targets, used either pure or enriched with crystalline silicon inserts, gives continuous control of both the refractive index and the optical bandgap of non-stoichiometric SiO_xN_y films, without any reactive gas or post-deposition annealing. By varying only the RF power (25 to 75 W), the deposition time (10 to 120 min) and the substrate temperature (room temperature or 300 °C), the refractive index measured by null ellipsometry at 632.8 nm and 70° was tuned from 1.41 to 2.11, covering almost the entire interval between SiO_2 (about 1.44) and Si_3N_4 (about 2.05) [2]. Over the same conditions the Tauc optical bandgap for indirect transitions spanned 2.17 to 3.09 eV. Energy dispersive X-ray analysis ties this tunability to film chemistry, since the normalized oxygen ratio O/(O+N) grows systematically with the bandgap, so that oxygen-rich films behave in a silica-like way while nitrogen-rich films approach Si_3N_4 [3]. A clear inverse correlation between refractive index and bandgap is also found, consistent with amorphous silicon-based oxynitrides and giving a simple design rule that connects composition, index and gap. High-index films (n up to about 2.1) with low roughness, obtained at high power and room temperature, are well suited for optical waveguides and antireflection coatings, whereas lower-index, wider-gap films work as dielectric and passivation layers, positioning insert-assisted SiON sputtering as a versatile, CMOS-compatible optical platform.

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ZIRCONIA/GRAPHENE ELECTROLYTES FOR SOLID OXIDE CELLS: EFFECTS OF GRAPHENE ORIENTATION AND FUNCTIONAL GRADING

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The development of advanced materials is essential to enhance the performance and durability of solid oxide electrochemical cells (SOCs). The most widely used electrolyte in these systems, cubic yttria-stabilized zirconia (8YSZ), provides excellent chemical stability and ionic conductivity under operating conditions. However, its intrinsic brittleness under thermal cycling (start-up/shut-down) and the need to lower operating temperatures remain key challenges. Recently, efforts have focused on developing 8YSZ-graphene composites that leverage the mechanical reinforcement and electronic conductivity provided by graphene while preserving the intrinsic ionic transport properties of zirconia [1]. When the graphene content remains below the percolation threshold, these electrolytes behave as mixed ionic–electronic conductors, thereby enabling an expansion of the electrochemically active region and potentially enhancing cell performance and reducing operating temperature.

In this work, 8YSZ–graphene electrolytes with preferential graphene orientation were developed to promote a cross-flow of ionic/electronic carrier transport. Additionally, functionally graded laminated electrolytes were designed, such that graphene-containing regions can be positioned adjacent to the anode upon cell assembly, minimizing thermal degradation in the oxidizing environment of the cathode. The materials were fabricated using conventional powder metallurgy and additive manufacturing techniques, with subsequent consolidation by Spark Plasma Sintering. The effect of graphene incorporation on the microstructure was analyzed, focusing on its homogeneous dispersion within the ceramic matrix and the structural integrity of the laminate interfaces. Mechanical properties were assessed by Vickers indentation, while interfacial integrity in laminated materials was evaluated through scratch testing. Electrical conductivity was characterized using electrochemical impedance spectroscopy to assess the influence of graphene on charge transport and on the ionic-to-electronic conductivity ratio. Impedance spectra were analyzed using equivalent circuit modeling and distribution of relaxation times analysis, allowing the identification of polarization mechanisms associated with the presence of graphene at ceramic grain boundaries and providing a more accurate description of ionic transport.

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Tribological performance of Ti-Al-N coatings deposited by vacuum arc

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We present the results of studies on Ti-Al-N coatings before and after they are subjected to heat treatment. These coatings were fabricated using an innovative Cylindrical Hot Refractory Anode Vacuum Arc (CHRAVA) system. The cathode design, consisting of a series of interchangeable rings, facilitated the easy adjustment of precursor compositions. Specifically, a complete cylinder was constructed using Ti rings, with Al rings strategically integrated in various sequences. Our analysis involved examining the coatings' structure, composition, and mechanical performance under wear conditions. X-ray diffraction identified a characteristic Ti-N structure, which evolved with the incorporation of Al. X-ray photoelectron spectroscopy further confirmed the presence of elements from the cathode rings and demonstrated an increase in Al content corresponding to the addition of Al rings. Additionally, tribological experiments on polished stainless-steel samples assessed the wear rate and coefficient of friction under different constant loads of 1, 2, and 5 N. The results were analyzed to understand the effect of increasing aluminum incorporation on the tribological performance of the coatings. The heat treatment was carried out at 700 °C for 2 hours, with a nitrogen flow of 2 sccm, and the same tests were performed to observe the changes.

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Study of Ion and Electron Energy Distributions in a Parallel-Plate Glow Discharge Using RFEA and OES

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Ion and electron energy and spatial distributions were investigated in a parallel plate argon glow discharge (100–250 mTorr) using a retarding field energy analyzer (RFEA) and optical emission spectroscopy (OES). The RFEA, composed of a negatively biased diaphragm (-50 V) and a collector swept from 0 to +100 V, was placed behind a grounded cathode, while the anode operated at 500-800 V. Plasma passed through an aperture in the cathode to the collector, allowing to obtain information of ion energy distribution from the I V curves. OES included the neutral argon lines at 750.4 nm and 811.5 nm, mainly associated with electron impact and ion-impact excitation, respectively. The 419.8/420.1 nm intensity ratio was used to estimate electron energy. It was found that maximum electron and ion energies were on the order of tens of eV, despite discharge voltages of several hundred volts. Also spatial emission profiles of the cathode and negative glow were analyzed in terms of particle interactions

References should be listed at the end using standard Chemical Abstracts Source Index (CASSI) terminology followed by **Year (bold)**, Volume and Pages. Put references in the text in brackets [1]. All participants are requested to use preferably Word for Windows and submit their abstract(s) via web-site as an attached file in Word-format.

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SYNTHESIS AND CHARACTERIZATION OF MAGNETOLUMINESCENT NANOARCHITECTURES Fe_3O_4@SiO_2@$NaYF_4$:Er^{3+},Yb^{3+}

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Magnetoluminescent nanoarchitectures integrate magnetic response and optical emission within a single entity, with potential applications in bioimaging and nanothermometry [1,2]. This work presents advances in the synthesis of Fe_3O_4@SiO_2@$NaYF_4$:Er^{3+},Yb^{3+}. Fe_3O_4 was obtained by ultrasound-assisted coprecipitation and subsequently coated with SiO_2 through the Stöber method, whereas the $NaYF_4$:Er,Yb matrix was independently prepared. The materials were characterized by vibrating sample magnetometry (VSM), X-ray diffraction (XRD), dynamic light scattering (DLS), Raman spectroscopy, and photoluminescence. As shown in Figure 1(a), Fe_3O_4 exhibited a magnetization close to ±45 emu g^{-1}, together with reflections consistent with a spinel phase and an average crystallite size of approximately 27 nm. After SiO_2 coating, the magnetization decreased to ±13–14 emu g^{-1} because of the magnetic dilution effect of silica, while the characteristic magnetic response of the core was retained, as observed in Figure 1(b). The $NaYF_4$:Er,Yb matrix displayed visible emission around 488–490 nm, highlighted in Figure 1(c), and Raman bands associated with the fluoride lattice, confirming its suitability as a low-phonon-energy optical component [3,4]. These results preliminarily validate the magnetic and luminescent components and support the subsequent integration of the complete system.

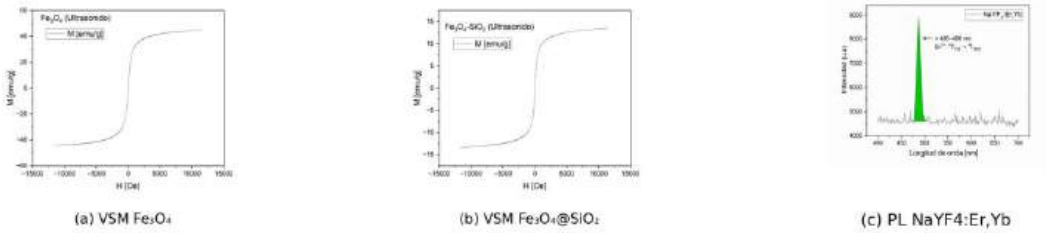

Figure 1. Magnetic response of Fe_3O_4 and Fe_3O_4@SiO_2, and emission of $NaYF_4$:Er,Yb.

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ROOM-TEMPERATURE STRONG-COUPLING ENGINEERING IN POROUS SILICON. FROM POLARITON CONDENSATES TO TAMM POLARITONS: AN OPEN POSSIBILITY FOR QUANTUM TECHNOLOGIES.

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Strong coupling is a quantum phenomenon amply searched nowadays, since formed hybrid light-matter quasiparticles enable deep subwavelength field confinement and strong intrinsic nonlinearities, promising the fabrication of revolutionary integrated nanophotonic devices [1]. Among the possible choices for the cavity formation, porous silicon is a material showing a well-stablished nanofabrication process and for which the porosity can be used to engineer refractive indexes [2], in such a way, that it can be designed as an optical component ranging from a Distributed Bragg Reflector (DBR) or a Fabry-Perot cavity, to any photonic crystal.

In this work, I present results in the realm of topological photonics regarding the formation of polariton condensates at room temperature using porous silicon photonic structures. We have followed two approaches: one using photonic quasicrystals, where a typical polariton condensate is observed, Fig. 1a) [3]. For the second one, we show how quasi-bound states (qBICs) in the continuum produce intense polariton coalescence, Fig. 1b) [4].

On the other hand, I also present results showing Tamm polariton formation, firstly, using gold in ultrathin DBRs, Fig. 1c) [5], and secondly, using silver in partially oxidized DBRs, Fig. 1d) [6].

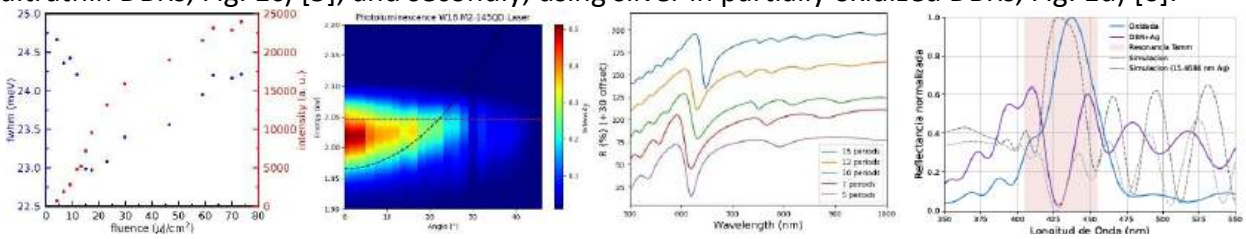

Figure 1. a) Fibonacci condensate, b) qBIC polariton coalescence; Tamm polariton using c) Au and d) Ag.

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Near-UV/blue photoluminescence in RF-sputtered silicon oxynitride thin films and the interplay between self-assembled silicon nanodomains and defect states

Arturo Rodríguez-Gómez[1], Luis Fernando Garrido-García[1], Ana Laura Pérez-Martínez[2], Alejandra López-Suárez[1] and María del Pilar Aguilar-Del-Valle[2]

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Achieving efficient light emission from silicon-based dielectrics is a long-standing goal for silicon photonics, where both quantum-confined nanostructures and intrinsic defects can act as radiative centers [1]. Here we report near-UV/blue photoluminescence (PL) from non-stoichiometric silicon oxynitride (SiON) thin films grown by RF magnetron sputtering of Si_3N_4 targets, pure or enriched with crystalline silicon inserts, at 300 °C and without post-deposition annealing. Under 325 nm He-Cd laser excitation, the films show a sharp emission peak near 3.2 eV (about 390 nm) together with a weaker, broader band extending toward 2.9 eV. High-resolution transmission electron microscopy reveals a transition from an amorphous matrix toward embedded Si-rich nanodomains about 2 nm in size when silicon inserts are used, and selected-area electron diffraction, indexed against Si and Si_3N_4 references, confirms the coexistence of cubic silicon and hexagonal Si_3N_4, with crystallinity and nanocrystal size growing as the RF power increases from 25 to 75 W. These structural fingerprints support a quantum-confinement picture in which excess silicon nucleates into quantum-dot-like inclusions. However, the same 3.2 eV feature is fully consistent with defect-related emission from oxygen-deficient centers, N-Si-O complexes and dangling bonds [2], and the 300 °C budget without annealing makes well-passivated sub-2 nm nanocrystals less likely, so we interpret the emission as an interplay of confinement and defect channels. Strikingly, while the effective optical bandgap is reduced systematically as the RF power increases, from 3.09 eV down to 2.17 eV, the PL intensity is non-monotonic and peaks at intermediate conditions, which reveals competing radiative and non-radiative pathways. These results identify insert-assisted SiON as a tunable near-UV/blue emitting layer for quantum-dot- or defect-based light sources [3].

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ELECTROCHEMICAL EVALUATRION OF CORROSION RESISTANCE OF A WEATHERING STEEL

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Weathering steel (also known as Corten steel) has been used in architectural installations and sculptures. This steel has certainly been used elsewhere in the world for highway barriers, due to its mechanical strength. In such cases, the use of de-icing salts introduces chlorides that jeopardize the protective integrity of the patina and the structure itself [1]. Regarding sculptures—such as Eduardo Chillida's "*El peine de los vientos*" (The Comb of the Wind) [2], located by the sea, or pieces in direct contact with water in fountains—chloride exposure can compromise the artwork's durability [3].

For this reason, it is essential to characterize the protective patinas of CORTEN steel and, if possible, to further stabilize them. This study evaluates both natural and artificially produced patinas using electrochemical tests (open-circuit potential, electrochemical impedance spectroscopy, and polarization curves) and metallographic observation via optical and electron microscopy, among other techniques.

Preliminary results indicate that the steel under study contains copper and chromium, which stabilize the natural patina. Polarization curves for rust-free, sanded CORTEN steel show passivation zones around 3–7 μA/cm² and a passivation range of 600 mV, indicating the potential for electrochemical passivation of this steel. The natural patina exhibits very stable OCP results during short-term exposure to the electrolyte, suggesting the presence of a stable, homogeneous layer; however, this does not appear to correspond to active behavior in the polarization curves.

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Characterization of sodium aluminosilicate by XRD, SEM and EDS for thermoluminescent ionizing radiation dosimetry

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Albite mineral is a plagioclase feldspar (sodium aluminosilicate, $NaAlSi_3O_8$) that exhibits luminescence under thermal and optical stimulation, which can be useful in applications such as geological and archaeological dating, environmental dosimetry, and identification of irradiated foods. Natural growth of albite minerals provides the formation of complex structural defects related to the presence of impurities and intrinsic defects [1]. For this reason, sodium aluminosilicate (NaAS, albite) was synthesized to investigate the formation of structural defects and their correlation with thermally stimulated luminescence, named thermoluminescence (TL), for its potential application in ionizing radiation dosimetry. NaAS samples were characterized using X-Ray Diffraction (XRD), Energy Dispersive X-Ray Spectroscopy (EDS), and Scanning Electron Microscopy (SEM) to analyze their crystalline structure, composition, and surface morphology. The crystalline structure of the samples showed the composition of 90% albite with a triclinic crystal system, 6% nepheline with a hexagonal crystal system, and 4% corundum with a rhombohedral crystal system. The EDS atomic composition of the samples exhibited Oxygen (61.06%), Sodium (7.33%), Aluminum (9.63%), Silicon (21.04%), Calcium (0.78%), and Potassium (0.16%). SEM images showed irregular and porous grains due to the evaporation of residual ethanol and water during thermal treatment. TL properties of dose-response, repeatability, and fading were investigated in NaAS samples exposed to Sr-90/Y-90 beta radiation. A wide TL glow curve composed of two overlapping peaks (96 and 210 °C), similar to that observed in natural albite minerals, was measured. TL dose-response has a linear behavior between 0.5 and 1000 Gy dose range. An acceptable repeatability of 2.7% was calculated after ten cycles of beta irradiation and TL reading. The anomalous fading, ubiquity characteristic of natural feldspar minerals, was observed at 24 h after irradiation of NaAS samples. At 30 days post-irradiation, the TL intensity decayed 54%, which is related to the release of electrons from shallow traps, i.e., thermally unstable energy levels at room temperature. Finally, the kinetic parameters of the TL glow curve (activation energy and frequency factor) were evaluated using a general order kinetics model.

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INFILTRATION OF Mg-Zn AND Mg-Ag ALLOYS INTO POROUS CERAMIC SCAFFOLDS OF BOVINE HYDROXYAPATITE

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Biodegradable magnesium implants corrode rapidly in physiological environments, leading to excessive hydrogen gas (H_2) production and a loss of mechanical properties, thus limiting their clinical application [1]. This study evaluated the effect of adding Zn and Ag on the corrosion behavior of magnesium compounds infiltrated into bovine hydroxyapatite (HA) to identify the best-performing composition for potential biomedical applications.

Master ingots of pure Mg, Mg-Zn1.5, and Mg-Ag1.5 (atomic weight percent) were obtained by inert-atmosphere melting. The HA was obtained from heat-treated bovine bone. The alloys were infiltrated into porous HA scaffolds in a controlled atmosphere. The compounds were characterized by XRD, pycnometry, SEM-EDS, microhardness, compression, electrochemical techniques (EIS and potentiodynamic polarization), hydrogen evolution, and tribological tests.
XRD results confirmed the formation of intermetallic compounds at the Mg/HA interface, indicating chemical interaction between the matrix and the ceramic. Mechanical tests showed that alloys with Zn and Ag had higher microhardness than pure Mg. Electrochemical tests in simulated biological fluid (SBF simulating blood plasma) [2] showed differences in corrosion response among the three compositions, which are currently being analyzed to correlate with hydrogen evolution and tribological behavior. Wear track profilometry further complements the characterization.

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Influence of the precipitating agent on the photocatalytic performance of $AlFeO_3$ synthesized by co-precipitation

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In materials science, synthesis conditions play a key role in controlling material characteristics such as size and morphology, which are directly related to functional behavior [1]. The co-precipitation method stands out due to its simplicity, cost-effectiveness, and controllability; in which precipitation conditions govern nucleation and growth, influencing the properties of the resulting material [2]. The choice of precipitating agent is a key synthesis variable that can alter the characteristics of the resulting solid. This study examines two precipitating agents (NaOH vs. NH_4OH) for the co-precipitation synthesis of aluminum ferrite ($AlFeO_3$) to determine which route enhances the material's photocatalytic activity. $AlFeO_3$ is a semiconductor with an optical response in the visible region and a bandgap near 2 eV, making it suitable for photocatalytic applications [3]. Oxytetracycline (OTC), a widely used antibiotic and emerging contaminant, was selected as a model molecule. The results show that both materials consist primarily of $AlFeO_3$ with an $\bar{R}3$ structure, with no structural differences observed based on the precipitating agent used. Similarly, the material's optical properties remained consistent, with bandgaps of 2.08 eV for NaOH and 2.13 eV for NH_4OH. In contrast, scanning electron microscopy (SEM) morphological analysis revealed more distinct differences: the material obtained using NH_4OH exhibited a more homogeneous morphology, whereas the sample synthesized with NaOH showed greater heterogeneity, featuring a mixture of polyhedral, prismatic, and elongated particles. Meanwhile, energy-dispersive X-ray spectroscopy (EDS) analysis revealed a more homogeneous elemental distribution of Al and Fe in the regions analyzed for the material obtained using NaOH, demonstrating that morphological homogeneity does not necessarily imply greater compositional homogeneity. Finally, preliminary photocatalytic experiments with the NaOH-synthesized material showed approximately 80% removal of OTC, as determined by HPLC. Overall, the results indicate that the nature of the precipitating agent influences the morphological and compositional characteristics of $AlFeO_3$. These differences could play a significant role in the materials photocatalytic behavior; therefore, a comparative evaluation of OTC degradation will make it possible to identify the characteristics that enhance photocatalytic activity and, consequently, determine the most suitable precipitating agent for $AlFeO_3$ synthesis.

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Homogeneous versus MOF-supported catalysis with a platinum tripodal complex for hydrosilylation of carbonyl compounds

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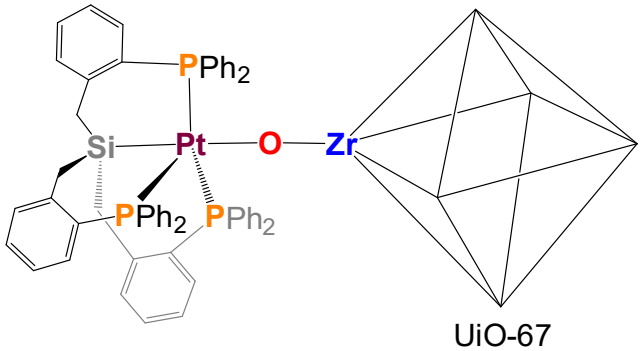

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Pt complexes derived from tetradentate ligands [HE(o-$C_6H_4CH_2P(C_6H_5)_2)_3$] (E = Si, Ge) were synthesized, resulting in a PtP_3EH-type complexes. Derivatives of these complexes, PtP_3SiCl and PtP_3SiMe were also accessed. PtP_3SiH proved to be an active catalyst for the hydrosilylation of aldehydes and ketones. The complex retains its catalytic activity once grafted onto a metal organic framework (MOF) and comparisons can be drawn between the homogeneous and heterogeneous systems, highlighting the advantages of MOF grafting. MOFs have a crystalline structure, low density, and thermal stability, allowing them to have extraordinary heterogeneous catalytic abilities[1]. Several MOF are used as supports enabling direct comparisons.

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INFLUENCE OF TITANIUM CONTENT ON THE PASSIVATION BEHAVIOR OF Ni-Nb-Ti METALLIC GLASSES

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The development of metallic materials with high corrosion resistance and long-term stability is critical for implant applications. Ni-based metallic glasses have attracted considerable attention due to their excellent corrosion resistance and mechanical performance [1-3]. In this work, the effect of Ti addition on the passivation behavior and passive film growth kinetics of $Ni_{50}Nb_{50-x}Ti_x$ (x = 10, 15, and 20 at.%) metallic glasses produced by melt spinning was investigated.

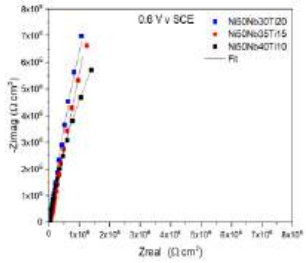

Figure 1. Nyquist diagrams for $Ni_{50}Nb_{50-x}Ti_x$ metallic glasses immersed in 3.5 wt.% NaCl at a) 0.6 V vs SCE.

Electrochemical characterization in 3.5 wt.% NaCl solution revealed a systematic improvement in corrosion resistance with increasing Ti content. The Nyquist diagrams (Figure 1) showed that $Ni_{50}Nb_{30}Ti_{20}$ metallic glass exhibited the highest corrosion resistance (Rtc), indicating a more protective and compact passive film.

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Halide-Induced Morphological Transformation of Silver Nanoprisms into Silver Nanospheres

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The optical properties of silver nanoparticles depend on their morphology due to localized surface plasmon resonance (LSPR). Silver nanoprisms are an excellent model system to study morphology-dependent plasmonic properties, as small changes in particle shape can lead to large spectral variations. In this work, the morphological transformation of silver nanoprisms (AgNPrs) into silver nanospheres (AgNPs) was investigated through their interaction with NaCl and KBr. The evolution of the nanostructures was monitored by UV–Vis spectroscopy and dynamic light scattering (DLS) to correlate the morphological changes with their plasmonic response. The results showed that exposure to halides induces a surface etching process that initiates at the high-energy vertices of the nanoprisms, promoting a gradual morphological transformation accompanied by a color change from blue to yellow [1,2]. These findings contribute to the understanding of halide-induced plasmonic transformations and highlight the potential of silver nanoprisms for halide sensing applications..[1–3].

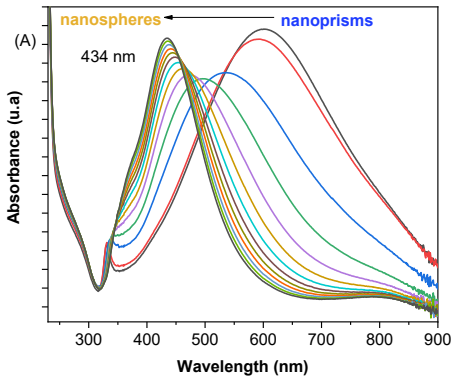

Figure 1. UV–Vis spectra showing the transformation of silver nanoprisms into silver nanospheres induced by NaCl and KBr.

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Exploring DyGdTbCoAl High-Entropy Alloys for Cryogenic Magnetic Refrigeration

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Rare-earth-based high-entropy metallic glasses (RE-HE-MGs) have attracted increasing interest as functional materials for low-temperature magnetic refrigeration due to their chemical complexity, tunable magnetic interactions, and the potential to combine broad magnetic transitions with reduced hysteresis. In this work, the structural, magnetic, and magnetocaloric properties of a DyGdTbCoAl RE-HE-MG were investigated. Metallic ribbons were fabricated by melt spinning. X-ray diffraction confirmed the formation of a fully amorphous structure, while scanning electron microscopy revealed a homogeneous morphology and uniform elemental distribution. Magnetic measurements using vibrating sample magnetometry revealed a coercive field of approximately 1.3 T at 2 K, indicating significant magnetic anisotropy at low temperatures. Field-cooled magnetization measurements under 5 mT revealed a Curie temperature of $T_c \approx 59$ K, consistent with a second-order ferromagnetic transition. The magnetocaloric response was evaluated from isothermal magnetization curves. For a magnetic field change of $\Delta H = 2.0$ T, a maximum magnetic entropy change of $|\Delta S_m| \approx 4.04$ J kg^{-1} K^{-1} was obtained near T_c. These results demonstrate that the DyGdTbCoAl high-entropy metallic glass exhibits a significant magnetocaloric response in the cryogenic-to-low-temperature regime, highlighting the potential of rare-earth-based amorphous multicomponent alloys for magnetic refrigeration and other energy-efficient solid-state cooling technologies.

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Abstract preparation

Vibrational Study of 4-NBT on Gold Using TERS

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Tip-Enhanced Raman Spectroscopy (TERS) is a characterization method that combines two powerful techniques: Raman spectroscopy and Scanning Probe Microscopy (SPM). Its principle is relies on the excitation of surface plasmons by a conductive tip, generating an electromagnetic field that locally enhances the Raman signal [1]. The incorporation of SPM allows not only the chemical signature of the system to be obtained, but also information about its physical morphology, thus providing a more complete characterization of the object under study [2]. It is worth noting that this technique does not necessarily require UHV conditions, as it can also be performed at atmospheric pressure, allowing its implementation in different experimental infrastructures.

In this work, a “homemade Raman” system was implemented using an optical lens arrangement, with which spectra from multiple samples have been obtained. The system is mounted on a movable base that allows displacement along the three axes, X, Y, and Z, as well as angular adjustment. This capability allows the geometry of signal incidence and collection in the TERS measurements to be modified. The Raman system was complemented with an ambient STM from Nanosurf, in which a gold tip was mounted. Gold tips were fabricated by electrochemical etching using a voltage controlled by an Arduino, with a gold wire as the cathode and a platinum ring as the anode. The quality of the resulting tips was verified by SEM.

Using this system, the 4-NBT molecule is studied after deposition onto a gold-on-glass substrate. The use of gold is important because, as a coinage metal, supports plasmonic excitations that can couple with the electromagnetic near field at the tip–sample junction, providing the local field enhancement required for TERS [3,4]. This system is used to study the vibrational response of 4-NBT under different illumination angles. Changing the angle modifies the geometry of signal incidence and collection, allowing its effect on the relative intensity of the different vibrational bands of the molecule to be investigated. Likewise, the spectroscopic response of the molecule is evaluated under different voltages applied through the gold tip, with the aim of determining possible changes in their intensity and position.

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Abstract preparation

Vibrational Study of 4-NBT on Gold Using TERS

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Tip-Enhanced Raman Spectroscopy (TERS) is a characterization method that combines two powerful techniques: Raman spectroscopy and Scanning Probe Microscopy (SPM). Its principle is relies on the excitation of surface plasmons by a conductive tip, generating an electromagnetic field that locally enhances the Raman signal [1]. The incorporation of SPM allows not only the chemical signature of the system to be obtained, but also information about its physical morphology, thus providing a more complete characterization of the object under study [2]. It is worth noting that this technique does not necessarily require UHV conditions, as it can also be performed at atmospheric pressure, allowing its implementation in different experimental infrastructures.

In this work, a “homemade Raman” system was implemented using an optical lens arrangement, with which spectra from multiple samples have been obtained. The system is mounted on a movable base that allows displacement along the three axes, X, Y, and Z, as well as angular adjustment. This capability allows the geometry of signal incidence and collection in the TERS measurements to be modified. The Raman system was complemented with an ambient STM from Nanosurf, in which a gold tip was mounted. Gold tips were fabricated by electrochemical etching using a voltage controlled by an Arduino, with a gold wire as the cathode and a platinum ring as the anode. The quality of the resulting tips was verified by SEM.

Using this system, the 4-NBT molecule is studied after deposition onto a gold-on-glass substrate. The use of gold is important because, as a coinage metal, supports plasmonic excitations that can couple with the electromagnetic near field at the tip–sample junction, providing the local field enhancement required for TERS [3,4]. This system is used to study the vibrational response of 4-NBT under different illumination angles. Changing the angle modifies the geometry of signal incidence and collection, allowing its effect on the relative intensity of the different vibrational bands of the molecule to be investigated. Likewise, the spectroscopic response of the molecule is evaluated under different voltages applied through the gold tip, with the aim of determining possible changes in their intensity and position.

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Structure, emission, optical and electrical parameters of Al doped $Mg_{0.20}Zn_{0.80}O$ films for TCO applications

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$Mg_xZn_{1-x}O$ alloys are important semiconductors for ultra-violet (UV) devices, which are required for a set of optoelectronics applications. A key limitation for the application of $Mg_xZn_{1-x}O$ films is their insufficient electrical conductivity. To improve the electrical conductivity, along with the crystal structure, optical, and emission characteristics, the $Mg_{0.20}Zn_{0.80}O$ films grown by spray pyrolysis on quartz or Si wafers were doped with Al elements (0.0-6.0 at%). The films are characterized by the wurtzite crystalline structure, a high transmittance of 80-95% and sharp fundamental absorption edges.

It was shown that Al doping up to 3.0 at% Al leads to the increase of the intensity of X-ray diffraction (XRD) peaks of the wurtzite crystal lattice, the increase of optical band gap and photoluminescence intensity, as well as the decrease of electrical conductivity in $Mg_{0.20}Zn_{0.80}O$ films. However, the doping with more than 3.0 at% Al stimulates the generation of acceptor-type defects due to beginning the self-compensation process in the films. This process is accompanied by structural re-orientation of films, along with the photoluminescence (PL) intensity decrease of near band edge (NBE) emission band and the intensity increase of new PL bands related to the carrier recombination via native donor-acceptor pair defects.
$Mg_{0.20}Zn_{0.8}O$:Al films are of interest for optoelectronic and photoelectronic applications as transparent conducting oxides (TCO) for ZnO-based displays, touch panels, ultra-violet (UV) photodiodes and other optoelectronic devices.

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DEVELOPMENT OF Mg-Li OPEN-CELL FOAMS FOR CO_2 CAPTURE

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The increase in global temperature, caused mainly by the increase in the concentration of greenhouse gases, such as carbon dioxide, is a global concern [1]. Alternatives have been sought to minimize this effect; one of them is the use of solid absorbents, among which are metal foams. Metal foams are porous materials that have porosity percentages above 50%, which gives them a greater surface area and a low density, characteristics that improve gas capture processes [2].

This study focuses on a systematic analysis of the $Mg_{100-x}Li_x$ (x=2,4) metal foams in solid solution. The master ingots were fabricated by casting in an induction furnace under an argon atmosphere. Subsequently, metal foams were obtained, seeking to obtain a percentage of porosity greater than 60%, by the infiltration method using NaCl as a preform. After melting, the preform was diluted; once the metal foam was obtained, XRD confirmed the presence of a solid solution. Scanning electron microscopy (SEM) and optical microscopy (OM) were used to study the microstructure and surface. In addition, with 3D reconstruction by X-ray microscopy (XRM) the type and percentage of porosity were studied. The low density of the foams and master alloys was determined by pycnometry, obtaining values lower than 0.66 and 1.76 g/cm^3, respectively. Subsequently, a surface oxidation process was carried out to form an oxide layer necessary for the capture process. The surface area of the samples after oxidation was evaluated by BET. Finally, studies with various relative humidity levels are expected to evaluate the capacity of Mg-Li metal foams in CO_2 capture processes.

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Instrumentation and Raman Spectral Measurements of Nanomaterials by Tip-Enhanced Raman Spectroscopy

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Tip enhanced Raman spectroscopy (TERS) is a powerful nanoscale technique that combines the advantages of nanometer topography images provided by the scanning probe microscopy (SPM) and the chemical fingerprint spectra of the constituents on the surface by optical Raman spectroscopy [1]. The nanometer gap formation between the tip and the metallic surface creates a well-positioned confinement cavity where the illuminated light on the tip is enhanced by interaction with the free electrons of the nanometer tip, therefore the existence of a high electric field interaction with the adsorbates on the surface. Despite its analytical power, the implementation of TERS remains experimentally demanding because it requires efficient optical excitation and collection within the restricted geometry imposed by a scanning probe microscope. Here we present the development and experimental validation of a modular Raman platform for lateral illumination specifically optimized for ambient TERS operation in combination with a scanning tunneling microscope (STM) and a mathematical model to represent the photon efficiency collection. Two optical system were redesigned to improve optical throughput and experimental flexibility and compared. Ambient TERS measurements were carried out using electrochemically etched gold tips and Au on Mica substrate were functionalized with 4-methylbenzenethiol and other organic molecules. Distinct near-field Raman spectra attributed to 4-methylbenzenethiol and chromium oxide were obtained. These results demonstrate that a laboratory-built modular Raman instrument can be transformed into a practical ambient TERS platform through careful optical and optomechanical optimization. The system provides a robust basis for future nanoscale chemical characterization and for the quantitative modeling of optical throughput and near-field Raman enhancement.

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FROM THE LABORATORY TO THE ENTERPRISE: NANOTECHNOLOGY WITH AN ENTREPRENEURIAL FOCUS.

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The academic journey, from undergraduate studies to the doctoral level, provides a comprehensive perspective on how scientific research, driven by global collaboration, can be translated into tangible societal benefits. Beyond theoretical frameworks, science possesses an immense potential to generate cutting-edge technology capable of fundamentally transforming our world; it is through applied knowledge that the tools which elevate our quality of life are forged. This disruptive impact is evidenced by the legacy of visionaries who redefined modern industry: Kamerlingh Onnes (helium liquefaction and superconductivity, 1908), Marie Curie (mobile radiography units, 1914), Ernst Ruska and Max Knoll (transmission electron microscope, 1931), Alan Turing (foundations of computer science, 1936), Robert Oppenheimer (atomic energy, 1945), John Bardeen (first point-contact transistor, 1947), Gordon Moore (foundational microprocessors, 1971), Shirley Ann Jackson (telecommunications and optical fiber, 1976), Gerd Binnig and Heinrich Rohrer (scanning tunneling microscope, 1981), Geoffrey Hinton (deep artificial neural networks, 1986), Shuji Nakamura (high-brightness blue LED, 1993), and Jennifer Doudna & Emmanuelle Charpentier (CRISPR-Cas9 gene editing).

The central objective of this talk is to demonstrate that rigorous scientific and academic development is a powerful catalyst for emerging technologies with direct applications in everyday life and the industrial sector. Aligning with this vision of transformative innovation, Dr. León Nataret has made an outstanding contribution to the manufacturing of graphenic materials. By pioneering a green chemistry approach, he has successfully eliminated the use of highly toxic and environmentally harmful reagents, such as $KMnO_4$, $NaNO_3$, and H_2SO_4. Instead, Dr. León Nataret has developed sustainable synthesis methodologies utilizing edible organic waste—specifically nopal and onion peels—as precursors for graphene production. This breakthrough proves that nanotechnology can be simultaneously disruptive, commercially scalable, and ecologically responsible.

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Characterization of Pigments in the Temple of Santiago Apóstol (18th Century), Tupátaro, Michoacán

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Science and art are two sides of the same coin. From the moment early humans left their mark on the walls of the Sulawesi caves in Indonesia to the present day, techniques and materials have evolved in tandem. More specifically, the techniques used with these materials serve as the bridge between science and art, reflecting the artist's era and environment.

This project identified and registered the pigments and binders used in the painted ornamentation of the eighteenth-century coffered ceiling (*artesonado*) and altarpiece at the **Temple of Santiago Apóstol** in the community of Tupátaro, Huiramba municipality. This site is under the custody of the National Institute of Anthropology and History (INAH) but remains active for Catholic worship. The objective was to determine whether the works are tempera paintings and to precisely identify the pigment types and the organic nature of their binders.

Following the selection of sampling points and collection, the materials were characterized using UV–Vis spectrophotometry (UV–Vis), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR). The results revealed the presence of goethite, calcium carbonate, and silica, with colagen identified as the organic binder.

USO DE TECNOLOGÍAS INNOVADORAS Y SUSTENTABLES PARA LA PRESERVACIÓN Y MANIPULACIÓN DE SISTEMAS BIOLÓGICOS EN LA INDUSTRIA MINERA

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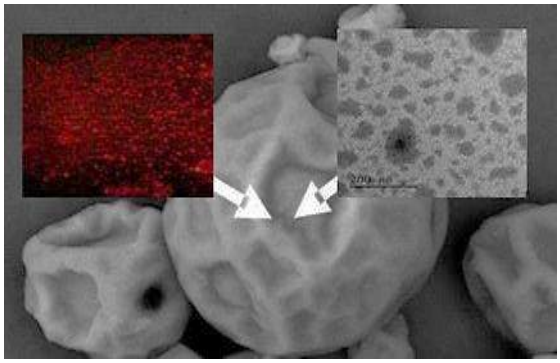
Los procesos biometalúrgicos constituyen alternativas prometedoras para la recuperación de metales y en la biorremediación de ambientes afectados por actividades mineras. Sin embargo, la implementación industrial de estas tecnologías continúa siendo limitada, principalmente por dos factores: los altos costos asociados al monitoreo de la actividad metabólica y la estabilidad genética de las bacterias durante los prolongados tiempos de operación [1]. Actualmente, se estima que, a nivel mundial, solo el 5% del oro y el 20% del cobre extraídos se obtienen mediante procesos de biominería, evidenciando la necesidad de desarrollar estrategias que favorezcan la conservación y disponibilidad de microorganismos de interés [2].



En este contexto, una estrategia prometedora para facilitar la manipulación y conservación de estos microorganismos es la microencapsulación. En este trabajo, se encapsuló *Acidithiobacillus thiooxidans* mediante secado por aspersión, utilizando diferentes biopolímeros como materiales de pared. Las microcápsulas obtenidas presentaron propiedades fisicoquímicas adecuadas para su almacenamiento, con actividad de agua (a_w) menor a 0.55 y humedad inferior al 10%. El análisis por microscopía electrónica de barrido mostró micropartículas esféricas, homogéneas y sin evidencia de colapso estructural, lo que sugiere adecuada estabilidad mecánica. Además, se alcanzó una supervivencia bacteriana de 1.4×10^9 cel/mL y una capacidad lixiviante del 95%. De manera destacada, las bacterias encapsuladas permanecieron viables durante más de dos años, garantizando su almacenamiento y disponibilidad para aplicaciones biohidrometalúrgicas a largo plazo. Estos resultados evidencian que la microencapsulación por secado por aspersión es una tecnología eficiente, escalable y sustentable para la preservación de microorganismos de interés en la industria, en particular contribuyendo al desarrollo de procesos biometalúrgicos más robustos y ambientalmente responsables.

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SUSTAINABLE METHODS STUDY AND DEVELOPMENT FOR THE PREPARATION OF BIODIESEL-D-LIMONENE-BASED BIOFUELS

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Globally, fossil fuels have represented an increasingly important source of energy contributing to industrial and economic growth. According to the Energy Transition Law in Mexico issued in 2015, a transition strategy was implemented to support the transition to cleaner technologies and fuels [1-3]. This research proposes the development of a sustainable biofuel production process involving the one-step (*in situ*) transesterification of *Ricinus communis* seeds using lemon citric oil or the terpene d-limonene as a green solvent in the presence of homogeneous (NaOH) or heterogeneous (CaO) catalysts. The citrus fruits acted in multiple roles in the *in situ* transesterification reaction: 1) functioning as extraction agents, 2) solvents, and simultaneously as a 3) biodiesel additive to obtain a biodiesel-d-limonene blend. The *in situ* transestrification of the seed was carried out using the NaOH catalyst (NaOH/oil = 1.2 wt. %) and CO catalyst (CaO/oil = 2.5 % wt.) at different oil/green solvent weight ratios (1:1 and 1:1.5), achieving a maximum conversion to free acid methyl esters of 99.99% during 3-6 hours reaction. The CaO could be reused in three reaction cycles in the presence of the green solvents, achieving conversions from 99 % to 42%. On the other hand, the biodiesel-d-limonene mixture (biodiesel/d-limonene weight ratios of 1:1 and 1:5) showed densities and kinematic viscosities with values within the EN 14214 and ASTM 6751 standards. The use of green solvents derived from citrus oils represents an alternative to the use of volatile organic solvents such as n-hexane, showing high efficiency in the extraction of oil from the *Ricinus communis* seed and in the production of biodiesel-d-limonene.

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Polymat Contributions

CHARACTERIZATION AND IN VITRO EVALUATION OF CHITOSAN/GUM ROSIN COATINGS ON *ESCHERICHIA COLI*

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In this study, coatings from chitosan, gum rosin and calcium oxide (CaO) microparticles synthesized from *Moringa oleifera* Lam. extract were characterized and their antimicrobial activity (colony forming units, CFU) against *Escherichia coli* was evaluated. The microparticles were characterized by transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDS), and dynamic light scattering (DLS) to determine their morphology, composition, and size distribution. From Fourier transform infrared spectroscopy (FTIR) the functional groups were identified. TEM analysis revealed spherical microparticles. EDS analysis confirmed the presence of oxygen (83.4%) and calcium (16.6%). DLS analysis indicated a particle size range between 246.1-284.1 nm. The coating formulations included chitosan (1 %), gum rosin (1 %, 2 %, and 3 %) and the CaO microparticles. The antimicrobial activity was evaluated at 24 and 48 h. The results showed that the coatings exhibited inhibitory effect on *E. coli* with a decrease in bacterial growth compared to the control (only chitosan). After 24 h, the formulations containing 2 % of gum rosin and the microparticles exhibited complete inhibition. After 48 h, the formulation with 3 % of gum rosin showed the lowest bacterial count (4.5 ± 1.29 CFU). The results suggests the potential of combining natural products and biodegradable materials as a future alternative for the elaboration of functional coatings to reduce *E. coli* on horticultural products.

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From Image to Decision: Advanced Characterization and Quality to Strengthen Industrial Innovation (Electron Microscopy at LUME)

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Manufacturing activities and industrial sectors in Mexico face increasingly demanding requirements for performance, reliability, and innovation in materials and components. Therefore, one of the main challenges is not only to increase manufacturing capacity but also to strengthen national capabilities to understand, characterize, diagnose, and improve both materials and industrial processes.

Electron microscopy is a key tool for studying the structure, composition, and behavior of materials at the micro-, nano-, and atomic scales. Its relevance to industry lies not only in its ability to produce high-resolution images but also in its potential to address specific questions, such as the causes of component failures, differences between conforming and defective batches, phase formation during processing, the presence of contamination, compositional distribution within components, phenomena occurring at interfaces, and microstructural changes that may explain variations in material performance.

Materials characterization by electron microscopy at the University Laboratory for Electron Microscopy (LUME) provides an effective approach to addressing technological problems. Case studies involving structural and chemical analyses will illustrate how an industrial problem can be translated into a working hypothesis, followed by the development of a characterization strategy and the generation of evidence that helps identify root causes and supports decision-making.

The reliability of results is a key consideration. Although an atomic-resolution image may have significant scientific value, its usefulness for industrial decision-making depends on factors such as sample representativeness and preparation, equipment calibration, identification of experimental artifacts, repeatability, reproducibility, traceability, and the technical competence of personnel. Adopting a quality culture and implementing management systems and standards such as ISO 9001 and ISO/IEC 17025 can help establish a common language between academia and industry, thereby strengthening confidence in characterization results.

University laboratories play an important role as technological partners for industry. In addition to providing access to specialized infrastructure, academic institutions contribute knowledge, methodologies, highly qualified personnel, and the expertise required to investigate complex problems. They also contribute to the training of specialized human resources and to the development of research and innovation projects.

The main challenge lies not only in observing materials at increasingly smaller scales but also in transforming those observations into reliable information, converting that information into knowledge, and using that knowledge to support better-informed technological and industrial decisions.

Fe_3O_4@GRAPHENE-MODIFIED CEMENT MORTARS AS FUNCTIONAL MATERIALS FOR Cu(II) REMOVAL FROM WATER

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The development of multifunctional cementitious materials that combine mechanical performance with contaminant removal is of growing interest for sustainable water-treatment applications. The use of cement-based materials modified with graphene and its derivatives provides an alternative approach for integrating nanoscale functionalities into structurally stable matrices [1]. In this work, Fe_3O_4@graphene (Fe_3O_4@G) nanocomposites were synthesized through a simple, environmentally friendly, and cost-effective approach and incorporated into cement mortars to investigate their effect on mechanical and morphological properties and their potential for heavy-metal removal. The Fe_3O_4@G nanocomposite was characterized by X-ray powder diffraction (XDR) and scanning electron microscopy (SEM), confirming the formation of the Fe_3O_4 phase and the dispersion of Fe_3O_4 nanoparticles (<100 nm) on graphene sheets. The nanocomposite was incorporated into cement–expanded perlite mortars at different dosages (1%, 2%, 3%, 4%, and 5% by weight), and the compressive strength was evaluated after 28 days of curing. The incorporation of Fe_3O_4@G increased the compressive strength of the mortars compared with the control, with the optimum mechanical performance obtained at 2 wt% Fe_3O_4@G, corresponding to a 59% increase in compressive strength. SEM analysis of the 2 wt% formulation revealed a denser microstructure and the formation of hydration products, including calcium silicate hydrate and ettringite within pores and microcracks, which may contribute to the observed mechanical enhancement. Based on this optimized formulation, the 2 wt% Fe_3O_4@G mortar was subsequently evaluated for Cu(II) removal from aqueous solutions. The mortar exhibited a Cu(II) removal efficiency of approximately 92% within the first 120 h, demonstrating that incorporating the nanocomposite provides not only mechanical reinforcement but also water-treatment functionality. These characteristics suggest the potential application of the developed mortars as permeable reactive materials or components of permeable reactive barriers [2,3]. Overall, the combination of structural integrity and contaminant removal capability highlights the potential of Fe_3O_4@G-modified cement mortars as multifunctional materials for heavy-metal removal and water remediation.

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ANTIBACTERIAL ACTIVITY OF ATACAMITE ($Cu_2Cl(OH)_3$) FORMED IN SITU DURING COPPER REMOVAL BY CEMENT–PERLITE MORTARS

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The development of multifunctional materials that combine contaminant removal with antibacterial functionality is of increasing interest in water treatment and environmental remediation. Copper-containing materials involving atacamite and paratacamite have previously demonstrated antibacterial activity against bacterial pathogens [1,2]. However, the antibacterial functionality of atacamite formed in situ on cement-based materials during Cu(II) removal remains underexplored. In this study, cement–perlite mortars were investigated for Cu(II) removal, with particular emphasis on the in situ formation of atacamite ($Cu_2Cl(OH)_3$) on their surface and the antibacterial functionality associated with the resulting Cu-containing surface layer. X-ray Diffraction (XRD) identified the formation of atacamite, while morphological characterization revealed the development of crystalline deposits on the mortar surface. X-ray Photoelectron Spectroscopy (XPS) was additionally employed to investigate the chemical state of copper at the treated surface. To evaluate the additional functionality generated during Cu(II) removal, antibacterial assays were performed against Escherichia coli and Staphylococcus aureus. Three Cu(II)-treated mortar formulations were evaluated using the agar diffusion method: cement–perlite without nanomaterials, cement–perlite containing magnetite, and cement–perlite containing the magnetite–graphene composite. All Cu(II)-treated mortars exhibited measurable antibacterial activity against both bacterial strains. For E. coli, inhibition-zone diameters of 16.55 ± 0.36, 17.15 ± 0.21, and 16.29 ± 0.31 mm were obtained for the three formulations, respectively. For S. aureus, inhibition zones of 10.52 ± 0.11, 9.96 ± 0.46, and 9.74 ± 0.26 mm were observed, respectively. These results suggest that the formation of an atacamite-containing surface layer during Cu(II) removal contributes to the antibacterial activity observed in the treated mortars, regardless of the incorporation of magnetite or the magnetite–graphene composite. This approach highlights the potential of Cu(II)-reactive cement-based materials to acquire an additional antibacterial functionality during contaminant removal, offering promising perspectives for the development of multifunctional materials for water treatment and environmental remediation.

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INFLUENCE OF AG IN ZN-AL ALLOY ON CRYSTALLITE SIZE PROCESSED CASTING AND MELT SPINNING

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$Zn-Al$ alloys with Ag additions of 1%, 4%, and 6wt% were synthesized under as-cast and rapid solidification conditions using the melt-spinning technique. The master alloys were prepared from high-purity Zn, Al, and Ag elements and cast under an argon atmosphere. Rapid solidification was achieved through a single copper roller liquid-quenching melt-spinning process. Structural and compositional characterization was carried out using $SEM{-}EDS$, XRD, and the Scherrer equation. The analysis revealed the presence of three main phases: Zn, $\alpha-Al$, and $\varepsilon-AgZn3$. The Ag content influenced the growth of the $\varepsilon-AgZn3$ intermetallic phase. The rapid solidification process significantly refined the microstructure of the $Zn-Al$-XAg alloys (X=1, 4, and 6 wt.%), producing more homogeneous and finer structures, with crystallite sizes reduced from the microscale to the nanoscale compared to the as-cast condition. This microstructural refinement and homogenization enhance the potential properties of these non-ferrous alloys for industrial applications. Moreover, the absence of an amorphous halo in the XRD patterns indicates a lack of non-crystalline phases, confirming a predominantly nanocrystalline structure. Selected Area Electron Diffraction ($SAED$) patterns further validate the crystalline nature of the alloys and reveal the presence of two distinct crystalline structures in the examined regions.

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Abstract preparation

Chemical synthesis and characterization of a fluorite/perovskite catalyst with the formula $Ce_{0.9}Gd_{0.1}O_{2-\delta}/Gd_{0.6}Sr_{0.4}FeO_{3-\delta}$

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The conditions for synthesizing the compound with the formula $Ce_{0.9}Gd_{0.1}O_{2-}\delta/Gd_{0.6}Sr_{0.4}FeO_{3-}\delta$ were determined using the combustion method via two approaches, conventional and modified. Characterization techniques were used to study and evaluate the structural, microstructural, and textural properties of the compounds, as well as their effects in the soot oxidation reaction (SOR) and the thermal decomposition reaction of ammonium nitrate (TDRAN). In these catalytic applications, the goal is to lower the reaction temperature. Finally, a catalytic evaluation of the catalysts synthesized by both routes of the combustion method was carried out. Using thermogravimetry, the SOR reaction temperature was determined to be 534 °C and the TDRAN reaction temperature 223 °C; these temperatures were achieved using the catalyst synthesized by the modified route. The kinetic parameters obtained were: activation energy of 60.1 kJ/mol and pre-exponential factor of 217.8 min^{-1} for SOR, and for TDRAN, 113.4 kJ/mol and 991,444 × 10^5 min^{-1}, respectively. The results obtained in the TDRAN were compared with results published in 2023 by Dave and Sirach in two separate studies. In the first study, it was reported that the maximum mass loss occurred at a temperature of 259.85 °C with an activation energy of 81.3 ± 7.7 kJ/mol, using nanocrystalline copper ferrite at 2% by weight as the catalyst [1], while in the second study, the maximum decomposition temperature was approximately 245.85 °C with an activation energy of 70.1 kJ/mol, using 2% $NiCuCr_2O_4$ as the catalyst [2]. Although the studies mentioned above do not use the same catalyst as the one presented here, the research conducted by Das and Pratihar in 2024 studied a similar structure, $Ce_{0.9}Gd_{0.1}O_{2-\delta}$ – $La_{0.6}Sr_{0.4}FeO_{3-\delta}$, in which they applied a one-step self-combustion method as the synthesis method, although its application was different [3].

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Characterization of the Micromorphology and Degree of Bonding of Sillar (Ignimbrite) qarry Waste via Scanning Electron Microscopy (SEM) as an Absorbent Porous Material and Eco-friendly Alternative for Arid-Zone Crops in the Arequipa Region

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Summary
Sillar, or ignimbrite, is an extrusive igneous pyroclastic rock formed by the cooling and consolidation of massive volcanic deposits; it is a material commonly used in construction in the city of Arequipa. This research aims to characterize the micromorphology and degree of welding of sillar quarry waste using Scanning Electron Microscopy (SEM) to assess its porosity and water-absorption capacity. The goal is to evaluate its potential as a support medium for low-water-consumption crops in the arid zones of the Arequipa region. SEM analysis revealed that the ignimbrite's pore structure—formed by gases trapped during lava cooling—makes it an ideal material for use as a surface mulch for low-water-consumption plants in arid areas. The morphological characterization demonstrated the material's high water-storage capacity, resulting from pores formed by ash and glass shards, which yields a capillary capacity of 36% to 41%. Crucially, the material retains its structural cohesion and does not dissolve when saturated by immersion or rainfall, offering a viable alternative for expanding agricultural frontiers in arid zones through low-water-consumption crops and reducing surface evaporation (the mulch effect). Quarry sillar waste was selected in average sizes of 25.4 mm and repeatedly washed with distilled water to remove native quarry salts; the material was then inoculated with humic acids, which serve as an organic stabilizer and soil conditioner, facilitating nutrient uptake by roots during sporadic irrigation.
Keywords: Sillar, degree of welding, porosity, morphology, extrusive igneous.

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INFLUENCE OF AG IN ZN-AL ALLOY ON CRYSTALLITE SIZE PROCESSED CASTING AND MELT SPINNING

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$Zn-Al$ alloys with Ag additions of 1%, 4%, and 6wt% were synthesized under as-cast and rapid solidification conditions using the melt-spinning technique. The master alloys were prepared from high-purity Zn, Al, and Ag elements and cast under an argon atmosphere. Rapid solidification was achieved through a single copper roller liquid-quenching melt-spinning process. Structural and compositional characterization was carried out using $SEM{-}EDS$, XRD, and the Scherrer equation. The analysis revealed the presence of three main phases: Zn, $\alpha-Al$, and $\varepsilon-AgZn3$. The Ag content influenced the growth of the $\varepsilon-AgZn3$ intermetallic phase. The rapid solidification process significantly refined the microstructure of the $Zn-Al$-XAg alloys (X=1, 4, and 6 wt.%), producing more homogeneous and finer structures, with crystallite sizes reduced from the microscale to the nanoscale compared to the as-cast condition. This microstructural refinement and homogenization enhance the potential properties of these non-ferrous alloys for industrial applications. Moreover, the absence of an amorphous halo in the XRD patterns indicates a lack of non-crystalline phases, confirming a predominantly nanocrystalline structure. Selected Area Electron Diffraction ($SAED$) patterns further validate the crystalline nature of the alloys and reveal the presence of two distinct crystalline structures in the examined regions.

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After rapid solidification, the microstructure clarifies the effect of Ag on the $ZnAl$ alloy, resulting in nanocrystalline alloys. The as-spun ribbons have a refined microstructure with homogenous dispersion of the $\eta-Zn$, $\alpha-Al$ phases, and Ag induces the presence of the inter-metallic $\varepsilon{-}AgZn3$. Adding Ag to the $ZnAl$ alloy will not reduce the crystallite size, but the rapid solidification process does. The crystallite size reduction at 99% of $\eta-Zn$, $\alpha-Al$ phases, and the inter-metallic $\varepsilon-AgZn3$ forming nanocrystallites in minimum sizes of 16.92 -1.57 nm from 250 μm calculated for alloys no-deformed.

Synthesis and characterization of PANI–MXene composites with varying MXene content for energy storage applications

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The development of composite materials based on conducting polymers [4] and MXene-type materials [1,2] constitutes an alternative for the study of materials oriented toward energy storage applications [3]. In particular, the incorporation of MXenes into a polyaniline (PANI) matrix [5] allows the influence of composition on the properties of the resulting materials to be studied. In this work, $Ti_2Al_{1-x}C$–TiC MXene-type material was incorporated into a PANI matrix via *in situ* oxidative polymerization in an acidic medium, using rapid mixing during the synthesis process [2]. Formulations with MXene contents of 25, 50, and 75% were prepared and labeled as P25, P50, and P75, respectively, in addition to PANI and MXene as reference materials.

The objective was to study the influence of MXene content on the capacitance properties of the composites and to generate information related to their potential application in energy storage systems.The synthesized materials were characterized by Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) to analyze their chemical and structural characteristics. The FTIR spectra showed signals associated with PANI and MXene in the different formulations, with spectral modifications observed as the MXene-type material was incorporated. Comparison of P25, P50, and P75 with the reference materials allowed the presence of both components in the composites to be identified and the changes associated with their incorporation to be analyzed. XRD characterization complemented the structural analysis of the obtained materials. MXene was successfully incorporated into the PANI matrix, obtaining composites with evident structural and morphological modifications, as well as the presence of agglomerations.

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Evaluation of Ti_3C_2 MXene/PANI nanocomposites as anti-corrosion coatings.

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Corrosion poses a serious problem due to the significant economic losses it causes and the risks it poses to health and the environment [1]. Polymer coatings are one of the most important protective measures because of their high effectiveness and low or no toxicity. Currently, the use of two-dimensional (2D) nanomaterials, such as Gr, BN, MOF, etc., are of interest in the field of corrosion protection, with Ti_3C_2Tx MXene standing out for its high conductivity and large surface area [2, 3]. Thus, the objective of this study was to synthesize Ti_3C_2 MXene/PANI-based nanocomposites at different concentrations to evaluate their performance as anticorrosive coatings in a 3.5% (w/w) NaCl solution. Ti_3C_2 MXene was synthesized via the acid etching method with HF. PANI and the nanocomposites were synthesized via in situ oxidative polymerization by rapid mixing. The coatings were formulated using an alkyd resin (RA) and were deposited onto 1018 steel substrates. FTIR and XRD analyses indicated the formation of the nanocomposites. SEM and EDS confirmed a uniform distribution of Ti_3C_2 MXene within the PANI network. EIS and Tafel tests demonstrated that the Ti_3C_2 MXene/PANI-based coatings exhibit superior anticorrosion properties compared to their base materials.

Table 1. Electrochemical parameters of Ti_3C^2 MXene/PANI-based coatings.

Sample	CR (mpy)	η_{PROT} (%)
RPANI	0.0091	84.01
RPMAX25	0.0061	91.75
RPMAX50	0.0058	93.39
RPMAX75	0.0045	94.91

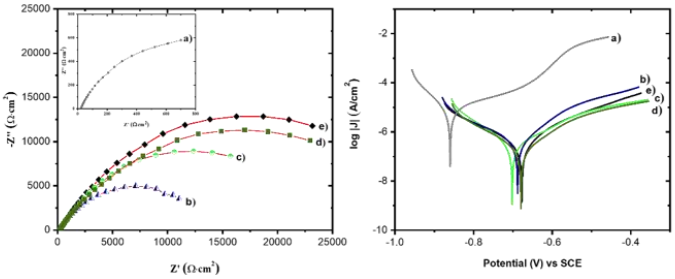

Figura 1. Nyquist diagrams and Tafel curves for: a) uncoated 1018 Steel (—), b) RPANI (—), c) RPMAX25 (—), d) RPMAX50 (—), and e) RPMAX75 (—).

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SYNTHESIS AND ANTIMICROBIAL EVALUATION OF ZnO:Pd FILMS VIA THE SOL-GEL METHOD

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Palladium (Pd)-doped ZnO films were prepared using the sol-gel method and the dip-coating technique. Zinc acetate and a palladium precursor were used and subjected to hydrolysis in methanol. Acetic acid was added to adjust the pH, while acetylacetonate and monoethylamine were used as stabilizing agents. Subsequently, the sol was deposited onto silica substrates through three dipping cycles. The structural, morphological, and antibacterial properties of the films were studied at three palladium concentrations: 1.0, 2.5, and 5.0 mol%. X-ray diffraction (XRD) results showed that, after heat treatment at 500 °C, the films exhibited a hexagonal crystalline structure. Atomic force microscopy (AFM) showed a homogeneous, smooth, and crack-free surface, with an average roughness of 18 nm (Ra = 18 nm), consisting of interconnected particles. The synthesized films exhibited antibacterial activity against *Escherichia coli* and *Pseudomonas aeruginosa*. The film with the highest Pd content, corresponding to 5.0 mol%, exhibited the highest antibacterial activity against *E. coli*, with a value of 64.07%. In contrast, against *P. aeruginosa*, the highest activity, 76.43%, was obtained with the film containing 1.0 mol% Pd [1].

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LIFE CYCLE ASSESSMENT OF SOLID OXIDE FUEL CELL MANUFACTURING: CARBON FOOTPRINT AND ENVIRONMENTAL HOTSPOTS

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Solid oxide fuel cells (SOFCs) are an energy conversion technology of considerable interest due to their high efficiency and fuel flexibility [1]. However, the use of specialized ceramic and metallic materials, together with high-temperature manufacturing processes, may generate significant environmental impacts [2]. This study assessed the carbon footprint of manufacturing an SOFC stack through an attributional Life Cycle Assessment (LCA) using a cradle-to-gate approach, in accordance with the principles established in ISO 14040 and ISO 14044. The functional unit was defined as 1 kW of nominal electrical capacity of a manufactured SOFC stack. The system boundaries included raw materials, ceramic and metallic components, electrodes, the electrolyte, interconnects, sintering, and assembly. The carbon footprint was estimated to range from 320 to 360 kg CO_2e/kW, with a representative value of approximately 330 kg CO_2e/kW. Energy consumption during manufacturing accounted for more than 85% of the total environmental impact, with the heat required for sintering and co-sintering identified as the main environmental hotspot. The results indicate that lowering sintering temperatures and reducing processing times, using thinner electrolytes, and increasing the recycled material content of interconnects are relevant strategies for reducing the carbon footprint of SOFCs [2,3].

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Characterization of hard FeB and Fe_2B layers formed by the pack boriding process on a 316 L stainless steel

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In the present work, the characterization of hard boride layers (FeB and Fe_2B) formed on the surface of an AISI 316 L stainless steel by a thermochemical treatment called pack boriding is studied. The treatment was carried out using temperature conditions of 850°C, 925°C, and 1000°C, with times of 2, 4, and 6 hours for each sample [1]. The boriding mixture used contains potassium tetrafluoroborate (KBF_4), boron carbide (B_4C), and silicon carbide (SiC). The process used techniques such as metallographic optical microscopy and scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD) [2]. Likewise, measuring instruments like a Vickers microhardness tester were employed to perform a microhardness profile, and an optical profilometer to measure the roughness of the treated samples [3]. The results showed that the ideal treatment conditions correspond to 1000°C for 4 hours. Crystalline phases corresponding to FeB and Fe_2B were detected. It was identified that the obtained hardness was 16 times higher compared to the untreated samples, and the profilometry observed that at higher temperatures, the layers are homogeneous and less rough.

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CHALLENGES AND OPPORTUNITIES IN THE DEVELOPMENT OF POLYMERIC NANOCOMPOSITE MATERIALS

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Nanotechnology focuses on phenomena happening at the nanoscale. This is a field that is rapidly expanding, centered on creating functional and intelligent materials and systems that can be adapted for industrial-scale use. The significance of this option is primarily attributed to its affordability, safety, cleanliness, and favorable cost-to-attributes ratio. Recently, polymer nanocomposites that integrate nanoclays and nanographite have received attention due to their superior characteristics, including dimensional stability, heat deflection temperature, gas permeability resistance, flame resistance, and mechanical strength, surpassing pure polymers or typical micro-composites. While research into clay-based composites dates back to the 1970s, Toyota was the first to bring a commercially viable nanocomposite to market in the 1990s. The mismatch between hydrophilic silicate layers and hydrophobic plastics spurred investigation into how clay particles could be exfoliated, distributed, and dispersed within the polymer matrix. A crucial step in creating polymer nanocomposites is ensuring a mixing process that fully integrates nanoparticles with the matrix; otherwise, the outcome is a poorly dispersed micro-composite. The extensive surface area of nanoparticles yields a material with characteristics differing from those of the original polymer. Nonetheless, ongoing production challenges encompass processing issues, particularly related to nanoparticle dispersion and distribution within the matrix, surface modifications, and inter-phase compatibility, all intensified by the nanoparticles' propensity to coalesce. These materials unlock new application potentials, and advancements in this field are anticipated to continue expanding steadily over several decades. This session will delve into raw materials, processing techniques, performance criteria, and the role of mixing in dispersing and distributing nanoparticles within the polymer matrix. In the final segment, applications under the circular economy principle, particularly the application of sargassum in nanocomposites, will be considered.

Desarrollo de una aleación Co-25Cr libre de níquel para la fabricación de stents coronarios

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Las enfermedades cardiovasculares son la principal causa de muerte en México, siendo el infarto agudo al miocardio (IAM) la causa más frecuente [1]. Este evento ocurre cuando las arterias coronarias se obstruyen por la acumulación de placa aterosclerótica, lo que reduce el flujo sanguíneo [2]. La intervención en casos de IAM requiere la implantación de stents coronarios para restablecer la función de la arteria coronaria [3]. Debido a lo anterior, se han desarrollado al menos cinco generaciones de estos dispositivos médicos [4,5] para mejorar su desempeño tanto mecánico como en términos de biocompatibilidad. Investigaciones recientes resaltan el interés de fabricar aleaciones libres de níquel para aplicaciones biomédicas [6,7], esto debido a la influencia negativa del níquel en el desencadenamiento de procesos inflamatorios [8,9]. En este contexto, este trabajo presenta tanto los resultados más relevantes con respecto al desarrollo de una aleación Co-25%Cr solidificada rápidamente libre de níquel como la ruta tecnológica empleada para la obtención de prototipos de stents coronarios.

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MULTIFUNCTIONAL THERMAL, ACOUSTIC, MECHANICAL, AND ENVIRONMENTAL PERFORMANCE OF AGAVE BAGASSE–GYPSUM BIOCOMPOSITES FOR SUSTAINABLE BUILDING INSULATION

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Abstract

Agricultural residues offer a sustainable alternative for developing low-carbon building materials with multifunctional properties. This study investigates gypsum-based biocomposites reinforced with Agave angustifolia Haw bagasse for thermal and acoustic insulation applications. Bagasse fibers of different lengths were incorporated into gypsum at various proportions and characterized by optical and scanning electron microscopy, thermal conductivity (ASTM D5334), acoustic absorption (ISO 10534-2), compressive strength (ASTM C39), and cradle-to-gate Life Cycle Assessment (ISO 14040/14044).

Microstructural analysis showed that the discontinuous gypsum–fiber interface generated an interconnected porous network that reduced heat transfer and enhanced sound dissipation. Fiber morphology significantly influenced density, porosity, and composite performance. The optimum formulation (50 wt.% gypsum–50 wt.% agave bagasse) achieved a thermal conductivity of 0.037 W m^{-1} K^{-1}, comparable to commercial insulation materials. Medium-fiber composites exhibited the highest volumetric heat capacity (1.158 MJ m^{-3} K^{-1}), while short-fiber composites showed the greatest thermal resistivity (791 °C·cm W^{-1}).

Acoustic tests demonstrated excellent sound absorption at medium and high frequencies, reaching coefficients of 0.93 at 2.5 kHz and 0.87 at 5 kHz. Compression strengths up to 2.20 kPa confirmed adequate mechanical integrity for lightweight, non-load-bearing insulation panels.

Life-cycle assessment indicated that partial replacement of gypsum with agave bagasse reduces embodied carbon, valorizes an abundant agro-industrial residue, and provides temporary biogenic carbon storage. These results demonstrate that agave bagasse–gypsum biocomposites combine competitive thermal insulation, effective acoustic performance, adequate mechanical strength, and reduced environmental impact, making them promising sustainable materials for low-carbon building applications.

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DEVELOPMENT OF A SUSTAINABLE AGAVE FIBER/NATURAL LATEX BIOCOMPOSITE FOR THE RESTORATION OF ERODED SMALL-SCALE WIND TURBINE BLADES

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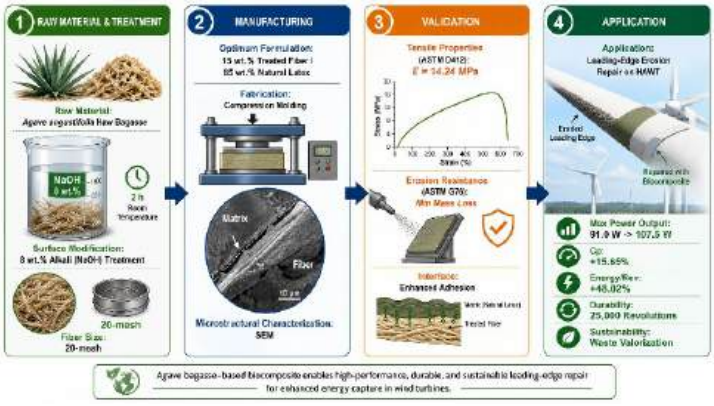
Abstract

The leading-edge erosion of wind turbine blades progressively reduces aerodynamic efficiency, increases maintenance costs, and generates large amounts of non-recyclable polymeric waste. This work presents the development and validation of a sustainable biocomposite based on Agave *angustifolia Haw* bagasse fibers reinforced with natural latex for repairing eroded small-scale wind turbine blades. Agave bagasse was chemically treated with an 8 wt.% alkali solution to improve fiber–matrix adhesion. Compression-molded specimens were manufactured and characterized following ASTM D412 tensile testing and ASTM G76 erosion testing. Microstructural evolution was examined by scanning electron microscopy (SEM), while the repaired blades were validated under real operating conditions using a horizontal-axis wind turbine. The optimum formulation consisted of 15 wt.% alkali-treated agave fiber (20-mesh) and 85 wt.% natural latex, yielding the highest elastic modulus (14.24 MPa) together with the lowest erosion-induced mass loss. SEM observations confirmed improved interfacial characteristics after alkali treatment, explaining the enhanced erosion resistance. Following gravimetric restoration of the blade profile, the repaired turbine recovered and surpassed its original aerodynamic performance. Maximum electrical power increased from 91.0 W to 107.5 W, corresponding to a 15.65% increase in the power coefficient (Cp) and a 48.02% improvement in energy harvested per rotor revolution. Durability testing over 25,000 rotor revolutions revealed no delamination, cracking, or debonding of the repaired region, demonstrating excellent structural integrity under centrifugal loading. These findings demonstrate that agave fiber/natural latex biocomposites constitute an environmentally friendly alternative for restoring wind turbine blades while reducing dependence on conventional synthetic polymers and valorizing agricultural residues, thereby contributing to more sustainable polymeric materials for renewable energy applications.



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Incorporation of persistent ZrO_2 into hydrogels for industrial applications

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Currently, organic materials exhibiting persistent luminescence have a wide range of industrial applications, such as flexible displays, portable electronic devices, and soft robotics [1]. Furthermore, hydrogels offer significant advantages over conventional polymers due to their biocompatibility, elasticity, and responsiveness to stimuli [2]. However, a drawback of hydrogels is that persistent emission is quenched under mechanical stress as non-covalent interactions break; consequently, hydrogel development poses a challenge for the industry [2]. This work presents the first 3D-printed hydrogels incorporating persistent ceramic materials—such as zirconium oxide (ZrO_2)—to prevent the disruption of covalent interactions and ensure that the persistence originates from the ceramic material. Luminescence measurements, mechanical tests, persistence data, and potential industrial applications for these materials are presented.

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Effect of the variation of growth factors of *Chlorella vulgaris* for biodiesel production in the presence of a heterogeneous catalyst

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Biodiesel is an organic fuel composed of monoalkyl esters, obtained through the transesterification of organic, algal, plant, or animal oils. Among the resources available for biodiesel production are microalgae, which are distinguished by their high productive potential, rapid growth, and low competition within the food sector.

Within this type of biomass is Chlorella vulgaris, a green unicellular microalga with a lipid content of 22.17% ± 0.46 [1]. One of the main challenges for industrial utilization is to increase lipid accumulation without significantly affecting biomass production. It has been demonstrated that environmental factors such as light intensity and nutrient availability [2].

Biodiesel production in the presence of heterogeneous catalysts has been strengthened in recent years. Heterogeneous catalysts such as layered oxides can be supported on biochar structures derived from organic materials such as sargassum, enhancing the structural and chemical efficiency of the catalyst itself and making it a material of great relevance for the transition toward green technologies [3]. Therefore, an evaluation of the influence of illumination and nitrogen limitation in the growth of Chlorella vulgaris will be carried out to increase lipid accumulation for its use in biodiesel production in the presence of a heterogeneous catalyst.

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COCOA SHELL-DERIVED CARBON MATERIALS FOR GLYPHOSATE RETENTION

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The design of functional carbonaceous materials from residual biomass represents a sustainable strategy for developing adsorbents with tunable properties for environmental applications. In this study, cocoa shell (CS) was used to produce biochar (BC) and H_3PO_4-activated carbon (ACT), and their physicochemical properties were related to glyphosate adsorption in both individual materials and agricultural soil. BC was produced by pyrolysis at 450 °C, whereas ACT was prepared by H_3PO_4 impregnation followed by thermal treatment at 850 °C. Thermochemical conversion increased the fixed carbon content from 19.4% in CS to 28.0% in BC and 72.4% in ACT. BC exhibited a BET surface area of 3.4 ± 1.2 m^2 g^{-1}, while ACT reached 1358.1 ± 14.8 m^2 g^{-1} and developed a micro–mesoporous structure with a BJH pore diameter of 5.2 nm. FTIR-ATR analysis showed the retention of oxygen-containing groups in BC and surface functionalities associated with H_3PO_4 activation in ACT. Adsorption equilibrium was reached within 24 h, with glyphosate adsorption of approximately 92.1% for ACT and 65.4% for BC. Incorporation of both materials into soil enhanced glyphosate retention compared with unamended soil, with the soil–ACT system showing the highest performance [1]. The maximum adsorption capacities estimated by the Langmuir model were 10.83 mg g^{-1} for BC and 7.77 mg g^{-1} for ACT. Despite its lower, ACT exhibited higher adsorption percentages, indicating that adsorption performance cannot be explained solely by surface area or maximum adsorption capacity [2]. Desorption reached approximately 74% in soil but decreased to only 6.3% and 5.2% for BC and ACT, respectively. Overall, glyphosate retention was governed by the combined effects of surface chemistry and pore structure [2,3]. The contrasting behavior of BC and ACT highlights the importance of tailoring both textural and chemical properties when designing biomass-derived adsorbents. These findings demonstrate the potential of cocoa shell as a sustainable precursor for functional carbonaceous materials aimed at reducing glyphosate mobility in agricultural soils.

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Linking Lignocellulosic Composition to Pore Architecture in KOH-Activated Carbons for Tartrazine Removal from Water

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The composition of lignocellulosic biomass influences the development of the porous structure of activated carbons and their potential as adsorbents [1,2]. This study evaluated the relationship between the chemical composition of residues from Lysiloma bahamensis (Lb) and Metopium brownei (Mb) and the surface properties of activated carbons obtained by KOH chemical activation for tartrazine removal from contaminated water. Lb showed a higher cellulose content (53.9%) and lower lignin content (21.7%) than Mb (44.7% and 24.9%, respectively), while hemicellulose contents were similar (14.9% and 15.2%). Lb also exhibited a lower ash content (0.34%) than Mb (1.1%). Both precursors had similar elemental carbon contents (46.8% and 46.7%, respectively), indicating that carbon content alone did not determine pore development. The biomasses were impregnated with KOH at an approximately 1:1 ratio and activated at 800 °C under nitrogen. N_2 adsorption at 77 K showed that both activated carbons developed micro- and mesoporous structures. The Lb-derived carbon exhibited a higher BET surface area (1265 $m^2\ g^{-1}$) than Mb (1065 $m^2\ g^{-1}$), as well as greater micropore volume (165.6 versus 138.2 mL g^{-1}) and external surface area (42 versus 36 $m^2\ g^{-1}$). Mesopore size distribution was evaluated using the BJH method. In contrast, Mb presented a larger average mesopore diameter than Lb (19.0 versus 13.2 nm), indicating greater mesopore widening. Overall, the results suggest that differences in lignocellulosic and mineral composition influence the response of each biomass to KOH activation, promoting greater microporosity and surface area in Lb [1,3]. The developed micro- and mesoporous structure and higher surface area are associated with enhanced tartrazine adsorption capacity, demonstrating the potential of these residues as precursors for activated carbons in water treatment.

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PEO/NASICON polymer composite solid electrolyte for sodium-ion batteries:effect of sodium salt on ionic transport

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Sodium-ion batteries are promising alternatives to Li-ion technologies for sustainable energy storage. However, efficient solid electrolytes remain a challenge. Polyethylene oxide (PEO)-based electrolytes offer flexibility but suffer from low room-temperature conductivity due to high crystallinity. Adding ceramic fillers like NASICON improves ionic transport.

In this work, PEO/NASICON composite solid electrolytes containing two different sodium salts – $NaPF_6$ and NaTFSI – were prepared by solution casting and compared. Membranes were characterized by XRD, FTIR, SEM, and electrochemical impedance spectroscopy (20–100 °C).

XRD confirmed NASICON presence and reduced PEO crystallinity with NaTFSI. FTIR showed stronger ion-polymer interactions for NaTFSI, indicating better salt dissociation. SEM revealed homogeneous ceramic particle dispersion. EIS measurements showed thermally activated transport. NaTFSI-based membranes achieved higher ionic conductivity than $NaPF_6$-based ones, attributed to lower ion pairing and increased amorphous PEO fraction.

These results demonstrate that sodium salt selection critically affects ionic transport. PEO/NASICON with NaTFSI is a promising candidate for safer solid-state sodium-ion batteries.

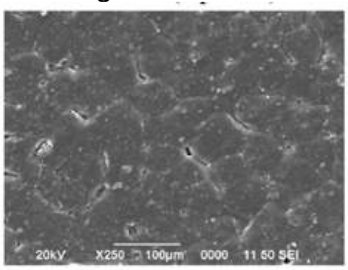

Figure 1. SEM micrograph showing homogeneous dispersion of NASICON particles in PEO matrix.

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Halophilic Archaea-Based Bioplastic for Agricultural Sensors with Hydrocarbon Bioremediation Potential.

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The intensive use of conventional petroleum-derived plastics in agricultural technology generates a critical accumulation of polluting waste in ecosystems. To address this issue, this work presents the development of a sustainable bioplastic synthesized from halophilic archaea, specifically designed for manufacturing protective enclosures for agricultural sensors. The archaeal polymers were obtained through controlled cultivation of halophilic microorganisms and formulated to create stable polymeric matrices without utilizing fossil additives. The resulting biomaterial demonstrated optimal mechanical properties for protecting electronic components in open-field conditions. Furthermore, preliminary testing indicates that this bioplastic possesses a high bioremediation potential, accelerating the degradation of petroleum hydrocarbons in contaminated soils and water bodies. This innovation offers a circular economy alternative that reduces the carbon footprint and actively mitigates environmental pollution in the agricultural sector.

Parameter	Value
Maximum Temperature Resistance	45ºC
Mechanical Properties	High flexibility and hardness (optimized via organic and plasticizing additives)
Impact Absorption	Excellent, capable of protecting electronic components against mechanical shock.
Water Resistance	Hydrophobic behavior
Hydrocarbon Degradation Rate	65% - 85%
Economic and Environmental Impact	30% increase in production value due to carbon footprint reduction

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Phenomenological Model for the Dynamic Superplastic Deformation Mechanism in a Zn-Al Eutectoid Alloy Modified with 2 wt% Cu

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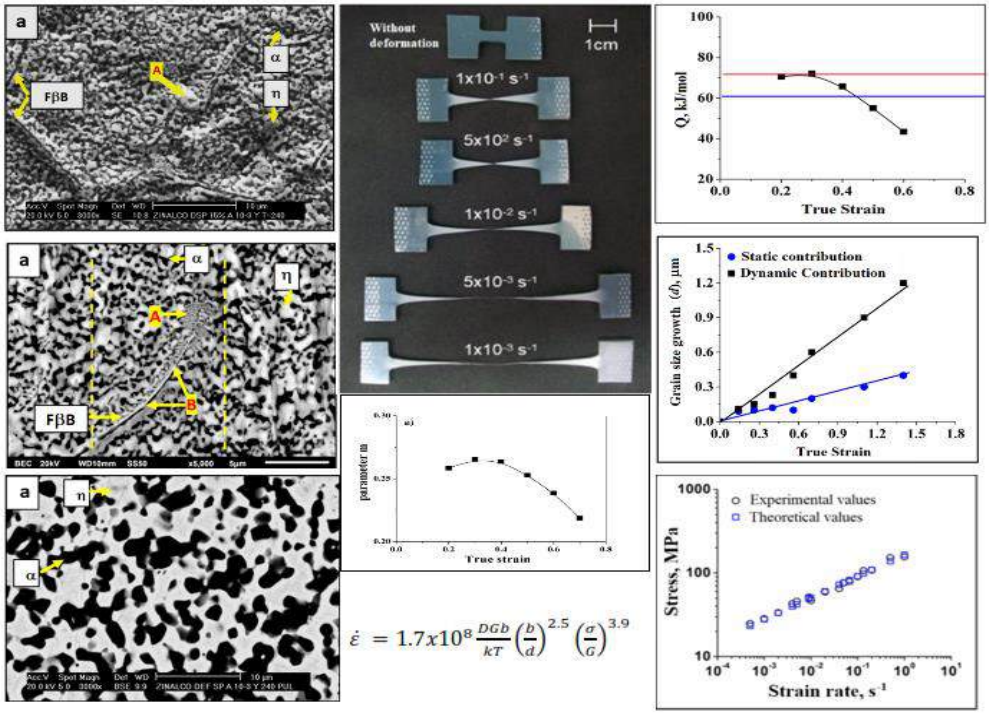
Abstact

In this work, superplastic behavior in tension for the Zn-21Al-2Cu alloy was reviewed as a function of: grain size, temperature and strain rate. The deformation mechanism was studied under conditions where the greatest elongation was reached, characterizing microstructural changes and analyzing the associated mechanical response such as the study of plastic stability. This analysis allowed us to propose a phenomenological model consisting of five steps for the mechanism of superplastic deformation under which dynamic conditions are involved for this alloy. In the first stage, an accommodation of the microstructure was observed, in the second stage sliding by individual grain boundaries (GBS) was activated, which provided the conditions for stationary plastic flow. In the third stage, GBS was hampered by the tendency of grain boundaries remaining from high temperature phase (FβBs) to align at 45°. This fact caused the onset of plastic instability.The fourth stage consisted of a transition in which there was competition between individual and cooperative GBS mechanisms, which increased plastic instability. In the last stage, the FβBs were aligned parallel to tensile direction, which favored the GBS, and an additional diffusion flow mechanism allowed partial recovery of stable plastic flow.



CONSTRUCTION MATERIALS AND SARGASSUM

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Sargassum is set to stay in the Caribbean. Scientists propose that its vigorous expansion is probably attributable to climate change, deforestation, and fertilizer use. However, research institutions and the business community have suggested that this scenario should not be considered a disaster.It presents an opportunity for creativity, allowing us to create jobs and well-being in affected communities, while also generating profits and economic benefits. Precise numbers regarding publications on sargassum and its industrial applications are not available. However, the evidence is unequivocal: there has been a significant growth in academic and business interests over the past five years, with particular acceleration since 2021. The strategy redefines biomass, currently considered a problematic environmental factor, as a valuable industrial opportunity. This investigation centers mainly on the valorization within the circular economy. Among the most notable methods are biofuel and energy generation, construction materials, and bioremediation (like altering asphalt and employing biochar to neutralize dyes in polluted water). Other strategies, high-value materials like hydrogels, crystalline cellulose, nanolaminates, bioplastics, alginates (food industry), fucoidans (medical applications), and similar. This paper illustrates examples of construction materials, including bricks, pavers, tiles, and interlocking concrete blocks, that have been formulated using sargassum after washing, drying, and grinding. Furthermore, the incorporation of cellulose nanolaminates—derived from sargassum using a physicochemical method—as an reinforcing element in concrete, as well as for thermoplastic and thermosetting polymer resins.

Structural and thermal characterization of citric acid-crosslinked hydrogels derived from post-consumer Denim

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Denim garments are hugely popular due to their durability and style. However, their mass consumption leads to a constant build-up of textile waste, as global production exceeds 4,000 million units a year [1]. This volume has a serious environmental impact: the manufacture of a single tonne requires 970 kg of cotton and 10,800 m^3 of water, whilst indigo dyeing generates 2 million tonnes of wastewater per year, as well as high CO_2 emissions and high energy consumption. As an alternative for value recovery, this study involved the extraction of cellulose powder from post-consumer denim via acid hydrolysis (HNO_3, 1 mol L^{-1}). The cellulose obtained was etherified using the Williamson synthesis to form carboxymethylcellulose (CMC), which was chemically cross-linked with citric acid to synthesize a hydrogel. The resulting materials achieved a swelling capacity of over 500 per cent, positioning them as potential water-retention agents and controlled-release systems for agricultural nutrients. The structure, composition and stability of the hydrogel were characterized using SEM, FTIR, rheometry and TGA. The process thus demonstrates the feasibility of transforming textile waste into functional materials with high added value, thereby promoting the circular economy and sustainable agriculture.

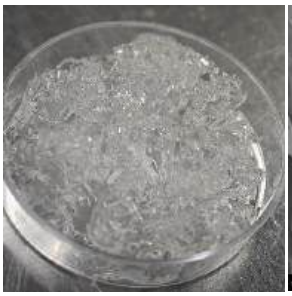

Figura 1. Swollen cellulose hydrogel

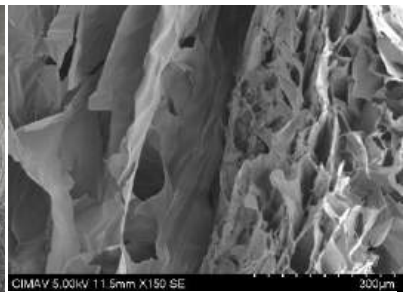

Figura 2. Scanning electron microscopy (SEM) micrographs of the showing surface.

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Thermomechanical simulation in a Gleeble system of similar and dissimilar butt welds of advanced TWIP and TRIP steels

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Solid-state butt welding is an efficient alternative for structural automotive components, as it preserves base metal properties by avoiding melting and filler metal addition, thereby mitigating severe microstructural alterations. This process facilitates the application of advanced high strength steels (AHSS), contributing to the manufacturing of lighter, safer vehicles with a reduced carbon footprint [1,2]. The study of joints between advanced TWIP (TW) and/or TRIP (TR) steels using this process has not yet been explored. Thus, this work evaluated the feasibility of butt welding between these steels using a Gleeble 563 thermomechanical simulator. An as-cast heat-treated TW steel and a thermomechanically processed TR steel were used. For the welds, two variants were compared, a joint formed by heating and compression, and another with post-compression heat treatment, allowing analysis of microstructural, structural, mechanical, and electrochemical behavior.

The results showed that similar TW joints present an HAZ with recrystallized and deformed grains, post heat treatment reduced hardness and increased ductility due to grain growth. In contrast, TR similar joints exhibited an HAZ with coarse and fine grain regions, showing a “V-shaped” hardness profile due to acicular ferrite at the interface. The multiphase microstructure of the TR steel increased strength compared to the base metal by 33% in the as-welded condition (1366 MPa) and by 20% after heat treatment (1299 MPa), the latter being the most ductile condition. In the case of the dissimilar joints between TW and TR steels, an intermediate behavior was obtained. The strengthening of the resulted weld is governed by TR steel and the ductility by TW steel, achieving an improved performance in the as-welded condition. Regarding corrosion behavior, a more stable passive layer was formed in the heat-treated weld condition, leading to a lower corrosion rate for both similar and dissimilar joints.

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EFFECT OF 2,5-DISUBSTITUTED 2H-TETRAZOLE FILM PERSISTENCE ON API 5L X70 STEEL IMMERSED IN A SALINE MEDIUM

L. A. Bello García[1,2*], A. Espinoza Vázquez[1], I.A. Figueroa Vargas[3], R. Orozco Cruz[1], G. E. Negrón Silva[4], A. Sánchez Eleuterio[4]

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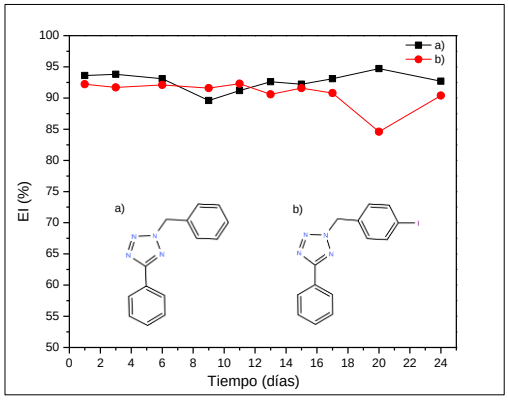

Figure 1. Variation in the inhibition efficiency of 2,5-disubstituted 2H-tetrazoles.

Corrosion of API 5L X70 steel in saline environments represents a significant concern for systems used in hydrocarbon transportation [1, 2]. In this study, the persistence of the film formed by two 2,5-disubstituted 2H-tetrazole derivatives on API 5L X70 steel immersed in 3% NaCl was investigated by monitoring the inhibition efficiency over a period of 24 days using electrochemical impedance spectroscopy (EIS). The results shown in Figure 1 demonstrate that compound 1a) exhibited inhibition efficiencies close to 90–95%, whereas compound 1b) showed a decrease to ~84.5% by day 20.

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Engineering Structural Defects in ZIF-8 to Modulate Arsenic Adsorption Sites: An Experimental and DFT Study

Aldo Arturo Castañeda Ramírez[1], Julio Cesar González Torrez, Victor Daniel Domínguez Soria, Ana Marisela Maubert Franco

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Arsenic contamination in groundwater remains a critical global threat, necessitating the development of high-capacity adsorbents. While Zeolitic Imidazolate Framework-8 (ZIF-8) is a prominent candidate due to its exceptional stability and porosity, its ideal crystalline structure lacks sufficient affinity for arsenic oxyanions, significantly limiting its removal efficiency in practical applications. This work addresses this gap through a multiscale approach, combining controlled experimental synthesis with Density Functional Theory (DFT) calculations to engineer structural defects that modulate adsorption sites.

By adjusting molar ratios and synthesis conditions, specific defects, including zinc (Zn) vacancies and dangling linkers, were successfully induced and validated through a correlation between experimental and simulated X-ray diffraction (XRD) and Fourier-transform infrared (FTIR) patterns Our results demonstrate that the inclusion of these defects drastically enhances the arsenic removal capacity, achieving up to 229.6 mg/g DFT calculations at the atomic level reveal that these structural irregularities transform previously passive regions into highly active centers.

The primary mechanism for this enhancement is the transition from weak physisorption in the pristine framework to a stable interaction involving electrostatic attraction and the formation of hydrogen bonds between the arsenic hydroxyl groups and the imidazole ring's nitrogen atoms. Specifically, the Zn vacancy was identified as the most energetically favorable and efficient defect for capturing As(III) and As(V). This study provides a rational basis for defect engineering in MOFs, highlighting their potential as tunable platforms for advanced water purification technologies.

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Determination of Arsenic in Mineral Waters by ICP-MS for Quality Control

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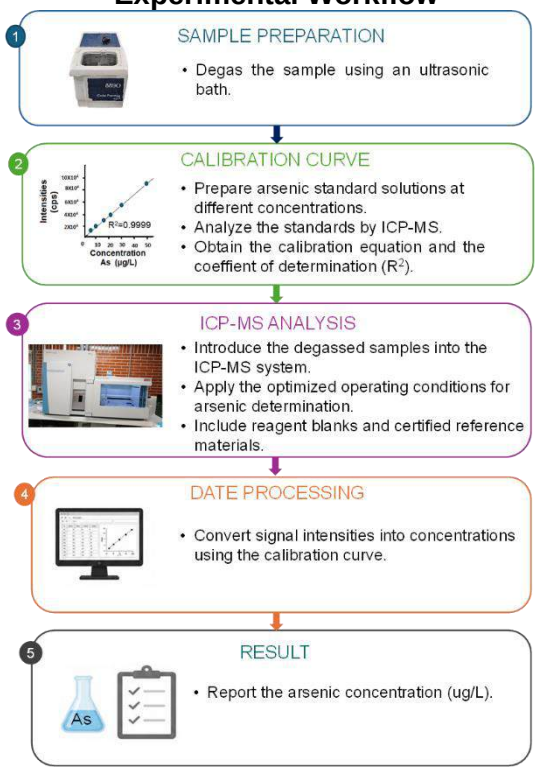
The reliable determination of arsenic at ultra-trace levels is essential to ensure the safety and quality of mineral waters. Arsenic is a naturally occurring toxic element widely distributed in the Earth's crust and may be present in groundwater and mineral waters as a consequence of geological processes [1]. Because inorganic arsenic species are classified as carcinogenic, their accurate determination is essential for regulatory compliance and public health protection [1, 2]. According to the Mexican regulation NOM-201-SSA1-2015, the maximum permissible concentration of arsenic in natural mineral water, mineralized water, carbonated water, and sparkling water is 0.01 mg/L (10 µg/L) [3]. Therefore, highly sensitive analytical techniques are required for the reliable quantification of arsenic at trace and ultra-trace levels.

In this study, inductively coupled plasma mass spectrometry (ICP-MS) with SQ-KED technology was employed for the determination of ultra-trace arsenic in mineral waters. The method showed excellent linearity, high sensitivity, and suitable analytical performance for the determination of arsenic at ultra-trace levels in mineral waters, its applicability for quality control.

Experimental Workflow



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THEORETICAL STUDY ON THE SUBSTITUTIONAL DOPING OF BORON NITRIDE MONOLAYERS FOR POLLUTANT ADSORPTION AND DETECTION

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Dichloromethane (CH_2Cl_2) and chloroform ($CHCl_3$) are colorless, highly volatile halogenated organic compounds characterized by a distinctive sweet odor and a density greater than water. Due to their chemical structure, they act as exceptionally potent solvents, easily dissolving fats, resins, plastics, and other organic substances that remain unaffected by water. Because of their extreme volatility, these chemicals rapidly release vapors into the environment. Inhalation depresses the central nervous system, leading to dizziness, nausea, and, at elevated concentrations, loss of consciousness or even death. Both chloroform and dichloromethane are highly toxic to the liver and kidneys and are currently classified as possible human carcinogens. Environmentally, because they are dense non-aqueous phase liquids (DNAPLs), soil spills seep deep into the ground and settle at the bottom of underground aquifers. This creates a persistent and highly toxic source of groundwater contamination that is exceptionally challenging and expensive to remediate.

Consequently, there is significant interest in developing novel materials capable of efficiently detecting and capturing these hazardous molecules. In this study, Density Functional Theory (DFT) was employed via the SIESTA code to investigate the interaction between these pollutants and a carbon-doped boron nitride monolayer. Our findings reveal adsorption energies ranging from 0.3 to 0.66 eV, with average adsorption distances varying between 2.02 and 2.75 Å. Furthermore, the adsorption process induces measurable changes in the electronic properties of the material, highlighting its promising potential as a foundational component for chemical detection devices.

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Abstract preparation

The effect of deep-sea into the corrosion behavior of X52 steel

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Jesus Rafael González-Parra[1], E. Lopez-Baltazar[1], A. Rodriguez-Gomez[2], J. Reyes-Gasga[2], A. Espinoza-Bautista[3], A. Barba-Pingarrón[1]

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The worldwide energy industry depends on great demand on hydrocarbons. The transport of crude oil is carried out using low-carbon steel with higher mechanical resistance catalogued as X52, X70 or X100. The X52 steel is widely used in Mexico for the transport and exploration of hydrocarbons. Since this steel is exposed to harsh environment is necessary to understand its corrosion phenomenon in deep-sea conditions [1]. On this research work we have used surface and electrochemical technique to compare the electrochemical corrosion behavior, semiconductor properties, composition and morphology of the oxide layer developed in atmospheric corrosion conditions and deep-sea corrosion conditions in ASTM synthetic sea-water. Results shown that the synergic effect of pressure and temperature determines the electrochemical response of the oxide layer that governs the corrosion resistance of the metallic X52 substrate. The crystallinity of the layer developed was modified by the hydrostatic pressure. Additionally, this results allow to support the fact that pressure is not the main control parameter for the corrosion processes in deep-sea conditions [2,3].

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Industriales, Aeroespaciales y Biomédicas" for their support during the development of this work.

Optical and Electronic Properties of the P35 Polyamide-Imide Isomer: An Experimental and TD-DFT Study

Salvador López Morales[1], Fausto Díaz Sánchez[2], Miguel Angel García Castro[2], Juana Deisy Santamaría Juárez[2], Zully Vargas Galarza[3], Edgar García Hernández[3].

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The design of polymers with tunable optoelectronic properties is a cornerstone for the development of electrochemical biosensors and advanced devices [1]. In this work, we present the synthesis and characterization of the polyamide-imide isomer designated as P35. The primary objective was to evaluate the direct impact of molecular architecture on the material's optical properties using UV-Vis spectroscopy coupled with quantum-chemical calculations. Experimentally, the optical energy gap (E_g^{opt}) was determined using the Tauc model, revealing that P35 exhibits a low energy requirement for photoexcitation. To elucidate this behavior at the electronic level, TD-DFT simulations were performed using the Solvation Model based on Density (SMD). Theoretical results demonstrated that the first singlet excited state (S_1) of P35 exhibits the lowest vertical transition energy (2.38 eV) while maintaining high oscillator strength [2], Figure 1.

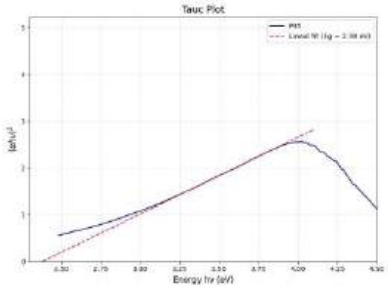

Figure 1: Determination of the optical band gap (*E*g) of polymer P35 by extrapolating the Tauc plot (*E*g = 2.38 eV)

This theoretical-experimental convergence confirms that the P35 isomer maintains an extended structural conformation that prevents self-folding, thereby maximizing the efficiency of the π-delocalization channel along the chain.

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VIABILITY STUDIO OF SUSTAINABLE AVIATION FUEL PRODUCTION FROM GRAPE POMACE VIA HYDROTREATMENT

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The bio-oil obtained from grape pomace through solid–liquid Soxhlet extraction is subjected to a hydrotreating process in a batch reactor under a hydrogen atmosphere. For this purpose, a bifunctional NiMo catalyst supported on SBA-15 and doped with Gallium at 3%. The NiMo active phase promotes hydrogenation and hydrodeoxygenation reactions, whereas the modified support provides acidic sites that promote cracking and isomerization reactions with selectivity toward sustainable aviation fuel range fractions.

The high surface area, porosity, and mesoporous structure of SBA-15 improve the dispersion of the active sites, which may increase the conversion of bio-oil into sustainable aviation fuel compared with catalysts having lower surface area and porosity.

Gallium incorporation aims to tune the acidity of the support toward isomerization and controlled cracking, promoting the production of branched biofuel hydrocarbons with physicochemical properties required for sustainable aviation fuels.

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BIOCOMPATIBLE ANTICORROSIVE COATING BASED ON POLY(GALLIC ACID) PLASTICIZED WITH GLYCEROL FOR STAINLESS STEEL

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Corrosion remains one of the main challenges affecting the mechanical and functional performance of metals and alloys, driving continued research into monitoring, prevention, and lifespan-extension strategies, particularly for metallic biomaterials requiring added biofunctionality[1-2]. Here, we report a low-cost, biocompatible coating based on protonated poly(gallic acid) (pPGAL) plasticized with glycerol, developed for stainless steel, one of the most widely used materials in the medical industry. pPGAL was synthesized via in situ oxidative polymerization using Trametes versicolor laccase, yielding a compound rich in primary amine ($-NH_2$), carboxyl (−COOH), and quinone groups that confer antioxidant activity, reduce corrosion rate, and support biocompatibility. Glycerol acts as a lubricant and filler, improving film flexibility and formation. Coatings were deposited by spin coating (750/1000 rpm,125 µL). Electrochemical impedance spectroscopy revealed a nearly threefold increase in coating resistance for the plasticized system (2.7 × 10^4 Ω.cm^2) compared to the non-plasticized control (1.3 × 10^4 Ω.cm^2), with maximum barrier performance observed between 3 and 5 h of immersion. These results position pPGAL as a promising, low-cost platform for functional biomedical coatings on stainless steel, which is currently being further optimized to enhance its long-term barrier stability and functional performance.

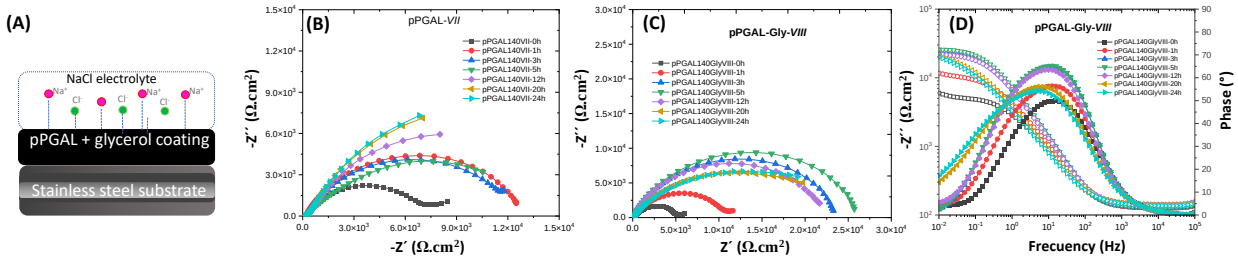

Fig 1. A) Arrangement of the plasticized coating; B) Nyquist plot for the non-plasticized coating; C) Nyquist plot and D) Bode plot for the plasticized coating.

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Influence of High-Energy Milling Time and Physical Crosslinking on the Properties of Post-Consumer Denim Hydrogels

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The textile industry is a major global economy driver, yet it generates substantial environmental impacts through massive waste production, particularly of post-consumer denim. Approximately five billion square meters of denim are produced annually; however, most end-of-life garments are landfilled or incinerated due to limited recycling technologies [1]. This results in the loss of valuable cellulosic resources and contributes to environmental pollution. To address this, this study demonstrates the synthesis and characterization of sustainable hydrogels derived from post-consumer denim. The recovered cellulose was subjected to high-energy milling at different time intervals, followed by cold dissolution and physical crosslinking using borax as a low-toxicity crosslinking agent at various concentrations. The resulting hydrogels exhibited a swelling capacity of up to 900%, highlighting their potential as water reservoirs and controlled nutrient delivery systems for agricultural applications. Microstructural, chemical, rheological, and thermal properties were confirmed using scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), rheological analysis, and thermogravimetric analysis (TGA). Overall, this work confirms the feasibility of upcycling textile waste into high-value functional materials, advancing circular economy principles and contributing to sustainable agricultural technologies.

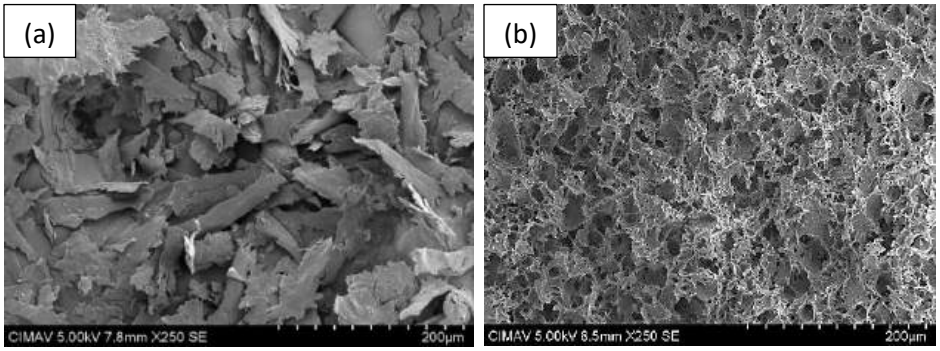

Figura 1. Scanning electron microscopy (SEM) micrographs of the (a) Denim after high-energy milling and (b) synthesized hydrogels, showing surface morphology at 250× magnification.

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LOW-COST ADSORBENTS FOR TOXIC METAL REMOVAL FROM WATER

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Water contamination by toxic metals and metalloids is a major environmental concern associated with untreated industrial, mining, and agricultural discharges. Cadmium (Cd), lead (Pb), arsenic (As), and mercury (Hg) are particularly concerning due to their persistence, toxicity, non-biodegradability, and bioaccumulation potential. This study evaluates low-cost natural materials and waste-derived adsorbents for the removal of Cd, Pb, As, and Hg from aqueous solutions, while promoting waste valorization and circular-economy strategies [1,2].

Peat, coal waste, banana peel, eggshell, calcium bentonite, and orange peel were selected based on their availability, chemical composition, and potential affinity for metal species. The materials were characterized by Fourier-transform infrared spectroscopy (FTIR), BET surface-area analysis, and point of zero charge (pHpzc) determination. Batch adsorption tests were conducted at an adsorbent dose of 7 g/L using independent solutions containing Hg (26 µg/L), As (26 µg/L), Pb (38 µg/L), and Cd (5.4 µg/L). The results showed substantial differences in removal performance among the tested materials. Banana peel achieved removal efficiencies of 81.8% for Pb and 79.1% for Hg, while eggshell reached 91.8% for Pb and 78.2% for Cd. Calcium bentonite showed the highest removal efficiencies for Pb (98.1%) and Cd (87.2%). Orange peel achieved 96.1% removal of Pb and 85.7% of Hg. Arsenic removal was comparatively low for most materials; however, banana peel exhibited the highest efficiency, reaching 56.5%. These findings demonstrate the potential of locally available natural materials and residues as affordable adsorbents for water remediation [2,3]. Their adsorption performance, low cost, and contribution to waste valorization support the development of sustainable treatment technologies, particularly for vulnerable communities and regions with limited access to conventional water-treatment infrastructure.

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Abstract preparation

Additive Manufacturing Using WAAM for Aluminum Alloys: Prospects and Challenges for Industrial Implementation

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Wire Arc Additive Manufacturing (WAAM) has established itself as one of the most promising technologies for producing large-format aluminum components, owing to its high deposition rate, high material efficiency, and reduced production costs. These advantages have driven its adoption in strategic sectors such as aerospace, automotive, marine, and energy. However, its industrial implementation still faces challenges related to porosity formation, columnar grain growth, anisotropy in mechanical properties, and the control of thermal cycles during manufacturing. In recent years, research has focused on developing new aluminum alloys, controlling heat input, optimizing deposition paths, and developing smart monitoring tools to improve the quality of manufactured components. This paper presents a review of recent advances and the main prospects for the industrial adoption of WAAM in aluminum alloys, highlighting its potential as an enabling technology for advanced manufacturing and Industry 4.0.

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METAL FOAMS: LIGHTWEIGHT ENGINEERING FOR A SUSTAINABLE FUTURE

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Metal foams represent a significant advancement in materials science by combining lightweight properties with high strength. Their porous structures mimics natural materials like bone or coral, offering efficient and sustainable solutions. They can be used in both structural and functional applications due to their low density—which significantly reduces component weight—as well as their high energy absorption capacity, making them ideal for safety applications. Additionally, they are recyclable, corrosion-resistant, and stable at high temperatures.These properties make them highly useful in sectors such as automotive and aerospace, where they improve energy efficiency, as well as in construction, biomedicine, and infrastructure protection. Innovation in their manufacturing drives more precise and sustainable engineering, positioning metal foams as key materials for developing cleaner and more efficient technologies in the future [1,2].

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Initial characterization of cellular concrete prior to accelerated aging in a custom-built chamber

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Autoclaved Aerated Concrete (AAC) is produced by mixing SiO2 (~55%), lime (~5%), cement (~20%), gypsum (~1%), and water (~19%), with the addition of aluminum powder (~0.1%) as a gas-generating agent. The mixture is placed in a mold where a chemical expansion reaction occurs, creating a matrix with millions of uniformly distributed air pores; this structure is responsible for the low density (300–1000 kg/m³) and the physicochemical properties of AAC. Subsequently, the material is molded, cut, and subjected to an autoclave curing process, where high pressures and temperatures induce the formation of hydrated calcium silicates, imparting the characteristic properties of AAC. Structural characterization was performed using X-ray diffraction to identify the phases formed, BET analysis to evaluate pore size distribution, and elemental analysis via X-ray fluorescence and confocal laser scanning microscopy.

An accelerated aging chamber prototype featuring humidity, temperature, and UV radiation controls was developed. The chamber is used to conduct aging tests on AAC (Autoclaved Aerated Concrete) using controlled cycles to evaluate physical, chemical, and microstructural changes under controlled environmental conditions: humidity levels of 60% to 90%, temperatures ranging from ambient to 100°C, and 465 nm UV radiation. The prototype is based on a modified electric oven integrated with a suite of sensors and electronic modules designed to control temperature, humidity, and UV radiation variables. This project was carried out at the request of Aircrete®, a company seeking a tool to study the deterioration of AAC materials under harsh environmental conditions to assess their durability.

The results obtained will contribute to the development of cellular concrete with greater durability, superior structural performance, and enhanced sustainability, while also generating useful guidelines for optimizing formulations and protective coatings within the construction industry.

Influence of Fe Content on Particle-Size Distribution and BCC Phase Formation in Mechanically Alloyed $Fe_x(CoCrMnMo)_{100-x}$ Powders

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Mechanical alloying is an effective solid-state route for producing compositionally complex alloys with refined crystalline structures [1,2], and powder-metallurgy processing allows further control over composition and microstructure [3]. Here we look at how Fe content shapes $Fe_x(CoCrMnMo)_{100-x}$ powders at 15, 30, 45, and 60 at.% Fe, mechanically alloyed for 10 h under argon. Powder morphology, particle-size distribution, chemical composition, and crystal structure were characterized by SEM, laser diffraction, XRF, and XRD. Fe15 and Fe30 showed bimodal particle-size distributions, with d_{90} values of 67.46 and 83.70 µm. Fe45 and Fe60, on the other hand, were mostly unimodal, with lower d_{90} values of 47.07 and 33.60 µm. XRD showed BCC-type solid solutions with crystallite sizes between 10 and 28 nm, with no FCC or intermetallic phases detected. Increasing Fe content improved granulometric uniformity and strengthened the Fe-type BCC contribution.

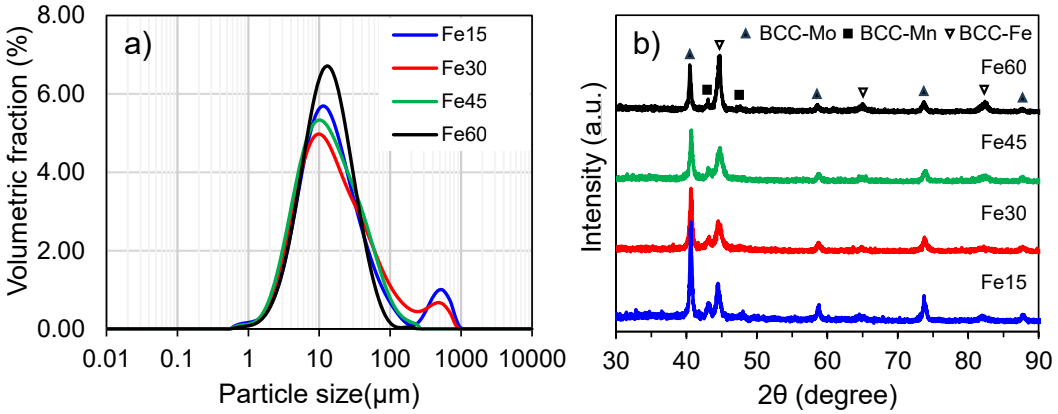

Figure 1. Effect of Fe content on the characteristics of mechanically alloyed: (a) particle-size distributions and (b) X-ray diffraction patterns showing the predominant BCC-type phases.

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Modifying the structural and electrical properties of CuO thin films via Mg doping using spray pyrolysis

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Copper oxide (CuO) is a p-type semiconductor with a narrow band gap (1.2-1.9 eV) [1] and moderate to high electrical and thermal conductivity, making it a promising material for energy storage, catalysis, gas sensing, etc. Despite their great potential, CuO nanostructures present limitations such as poor electrical conductivity, unfavorable optical properties, and lower catalityc activity. To overcome these drawbacks, the incorporation of foreign metal ions into the CuO lattice has proven to be a viable approach [2]. The Mg-doped CuO thin films were deposited by the spray pyrolysis technique on silicon and glass substrates at constant temperature of 350ºC with the different Mg doping concentrations (0.0, 5.0, 10.0, 15.0 and 20.0 % at.). XRD spectra demonstrated that CuO and Mg-doped CuO thin films showed a monoclinic structure. As the percentage of Mg increased, the XRD peaks shifted to slight greater angles, due to the almost equal ionic radii of Mg^{2+} (0.72 Å) and Cu^{2+} (0.73 Å) [3]. The XRD intensity increased up to 10.0 at% Mg content sample, and then decreased for the rest of the samples, indicating the beginning of the unit cell destruction process [4]. SEM images revealed the formation of nanocrystals whose radius decreases from 52.5 to 31.5 nm with increasing Mg content up to 20.0 at%. EDS analysis confirmed the presence of Mg into the CuO thin films. The decrease in nanocrystal size with increasing Mg content is expected to induce a widening of the optical band gap.

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Severe Plastic Deformation of Al–Li Alloys for Aerospace Applications: Opportunities in Mexico

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The increasing demand for high-performance lightweight materials in the aerospace industry has driven the development of aluminum-lithium (Al–Li) alloys, particularly third-generation systems such as AA2099, due to their superior strength-to-weight ratio, enhanced stiffness, and improved fatigue resistance. These properties are critical for high-speed aircraft operating under extreme conditions.

This work presents an integrated materials science approach applied to industrial manufacturing, focusing on the development, processing, and evaluation of Al–Li alloys in Mexico. Al–Li alloys were produced via gravity casting using high-purity elements with controlled lithium content (1.8–3 wt.%). Subsequently, Severe Plastic Deformation (SPD) using Equal Channel Angular Pressing (ECAP) refined the microstructure, promoting ultrafine grain formation and improved mechanical properties.

Aerodynamic simulations of a NACA 64A204 airfoil under supersonic conditions (Mach 1.2–3.0) revealed shock waves, pressure gradients, and thermal effects representative of high-speed flight. A specialized setup was designed to evaluate the structural dynamics under vibration conditions, following established design standards for a high-speed structure, focusing on the leading-edge.

Results demonstrate that integrating advanced processing techniques significantly enhances the performance of Al–Li alloys for aerospace applications. This work also highlights the strategic opportunity for Mexico to strengthen its capabilities in advanced materials manufacturing and reduce technological dependence.

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Integrated Pilot Plant for Pharmaceuticals Removal from Domestic Sewage

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Abstract

To address the growing water pollution in Mexico City, an automated and fully controlled three-stage pilot plant integrating Coagulation-Flocculation, Methanogenesis, and hybrid Advanced Oxidation Processes (AOP) was evaluated at the San Juan Ixhuatepec WWTP to remove recalcitrant pharmaceuticals (ciprofloxacin, cefadroxil, sulfamethoxazole, and carbamazepine) from domestic wastewater. Primary clarification via coagulation-flocculation operating under an optimal 1:1 coagulant-to-flocculant ratio effectively eliminated suspended solids, generating a clear effluent and reducing the initial total organic carbon (TOC) load from 1200 mg L^{-1} down to 200 mg L^{-1}. Subsequent anaerobic biotransformation in a UASB reactor—operating with a specific methanogenic sludge activity of 2.4 mg CH_4-COD/mg VSS L day validated through FTIR gas monitoring—biodegraded complex parent molecules into smaller, less hazardous metabolites while decreasing ionic concentrations of NO_3^-, SO_4^{2-}, and PO_4^{3-}. By sequentially coupling the methanogenic effluent directly into the electro-AOP system operating under automated process control at 30 mA cm^{-2}, a flow rate of 5 L min^{-1}, and 0.2 M salinity, the three continuous processes driven by hydroxyl radicals plummeted the TOC load further to 65.5 mg L^{-1}, confirming the remarkable mineralization capability of the integrated system. Overall, this controlled automated sequential physicochemical, biological, and advanced oxidation process configuration demonstrates superior organic pollutant degradation, offers promising energy recovery viability through biomethane production, and establishes a robust technological framework capable of delivering tailored treatment strategies customized for specific effluent compositions toward industrial scaling and sustainable wastewater reclamation in polluted urban basins.

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From Home to the Lab: The Journey of an Idea.

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Science is everywhere, and to delve into it, all that is needed is a simple idea. An everyday observation, perhaps in the tranquility of our home, that awakens in us the urge to solve a problem. And if we delve deeper, a genuine interest arises in solving a problem or even innovating and developing new materials. Depending on our background, a wide range of options can emerge to tackle this problem, and it is right here where we reach a turning point and take a great leap to go from an almost imperceptible question to the rigor of applying the scientific method, where the possibilities are as vast as our curiosity, being able to generate frontier knowledge, the pillar of our postgraduate studies, or reflecting in scientific productivity. Whatever the case may be, the main barrier is usually the budget we can allocate to research, and it is here where our ingenuity can help us overcome this barrier, provided we have the technical and theoretical solidity necessary to support, defend, and deeply understand the science we are creating. In our case, this curiosity allowed us to develop projects in different areas such as nanomedicine, environmental remediation, smart textiles, flexible electronics, advanced ceramics, and bone regeneration, enabling us to participate in different scientific events and, finally, the creation of our Instituto de Nanotecnología Aplicada (INA). In this talk, we will discuss the synthesis of various materials using easily accessible resources for their application in diverse areas, and their impact on the scientific community.

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Incorporation of persistent ZrO_2 into hydrogels for industrial applications

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Currently, organic materials exhibiting persistent luminescence have a wide range of industrial applications, such as flexible displays, portable electronic devices, and soft robotics [1]. Furthermore, hydrogels offer significant advantages over conventional polymers due to their biocompatibility, elasticity, and responsiveness to stimuli [2]. However, a drawback of hydrogels is that persistent emission is quenched under mechanical stress as non-covalent interactions break; consequently, hydrogel development poses a challenge for the industry [2]. This work presents the first 3D-printed hydrogels incorporating persistent ceramic materials—such as zirconium oxide (ZrO_2)—to prevent the disruption of covalent interactions and ensure that the persistence originates from the ceramic material. Luminescence measurements, mechanical tests, persistence data, and potential industrial applications for these materials are presented.

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OPTOELECTRONIC SYSTEM BASED ON SENSORS WITH ZnO:Al NANOSTRUCTURES FOR ATMOSPHERIC OZONE MEASUREMENT

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Ozone (O3) is a triatomic molecule composed of oxygen atoms. It is a naturally occurring component of the atmosphere, found in low concentrations, and is vital for life. Most ozone is located in the upper atmosphere, at ground level. High concentrations of ozone are an air pollutant that can have harmful effects on human health. Zinc oxide is a wide band gap semiconductor, which has attracted great attention over the last two decades due to its interesting optical properties, important for optoelectronic applications in blue and UV light emitting devices, photodiodes, solar cells and in high temperature electronics. The high exciton binding energy (60 meV) in ZnO promising a bright exciton emission at room temperature. High optical transmittance in the visible spectral range and significant electrical conductivity have drawn attention to ZnO NC films. Ultrasonic spray pyrolysis (USP) was applied to obtain the ZnO:Al films. The optoelectronic system designed for atmospheric ozone measurement is made up of the following elements: a solar tracker with stepper motors controlled by a PID, the sensor containing a ZnO:Al nanostructure-based photodiode with a collimating lens, ESP32 microcontroller, and the data transmission system with an interface to a laptop whit MatLab. An optical filter is required to allow only light at a wavelength of 315 nm to pass through so that the photodiode can measure the light intensity at this wavelength. For this purpose, a ZWB1 color optical filter was selected, which allows ultraviolet radiation at a wavelength of 315 nm to pass through.

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MICROWAVE-ASSISTED GREEN SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES FROM TOMATO PEEL EXTRACT

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Green technologies are increasingly in demand today, making the synthesis of different nanoparticles highly important. These nanoparticles offer a wide range of applications, including pharmaceutical, wastewater treatment and biosensing [1].The synthesis of silver nanoparticles (AgNPs) using aqueous plant extracts is gaining increasing relevance because AgNPs are of great interest due to their wide range of potential applications arising from their unique properties, while this synthesis method is preferred because it is less costly, safer, and more environmentally friendly [1]. Microwave-assisted synthesis of nanomaterials enables better control of the synthesis conditions, resulting in more crystalline AgNPs with a narrower size distribution, smaller particle sizes, and shorter reaction times [2]. In this study, silver nanoparticles (AgNPs) were synthesized through a facile and environmental-friendly procedure using the aqueous peel extract of tomato (*Solanum lycopersicum*) as an effective stabilizer and reducing agent. The investigation of the optimal synthetic conditions for AgNPs was achieved at 2 mL of the extract, 10 mM of $AgNO_3$, 130 $^{\circ}$C and 15 min of reaction time. Analytical techniques comprising UV-Vis absorption spectroscopy was used to confirm the AgNPs in the solution, FTIR spectroscopy was conducted to identify the potential functional groups (-OH, C-H, C=C, C=O) of biomolecules in the *Solanum lycopersicum* extract, which may have participated in the reduction of Ag^{+} and stabilizing of AgNPs. Energy dispersive spectroscopy (EDS) results revealed the presence of elemental AgNPs and scanning electron microscopy (SEM) were performed to identify size and morphology. Moreover, the average hydrodynamic size, polydispersity index (PDI) and the zeta potential also were evaluated. In conclusion, the results obtained suggest that it is possible to rapidly produce stable AgNPs using a low-cost, microwave-assisted green synthesis method.

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IMPLEMENTATION OF AI AND ULTRASOUND IN CANCER SCREENING: RESULTS IN LESS THAN A MINUTE WITH SONOSPECTRAL.

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Cancer represents one of the greatest challenges for contemporary public health. According to recent data from the International Agency for Research on Cancer (IARC), approximately 20 million new cases and 9.7 million deaths were recorded worldwide in 2022 [1]. It is projected that by 2050, incidence will increase by 77%, reaching 35 million new annual cases due to population aging and growth [2]. Given this scenario, early detection is a critical factor in reducing mortality and the costs associated with late-stage treatment. However, current screening methods tend to be specific to a single cancer type, costly, and reliant on long turnaround times that delay the start of treatment.

This work presents a national technological innovation that integrates the interdisciplinary implementation of ultrasound and artificial intelligence for cell characterization. The device employs high-frequency ultrasonic transducers to characterize samples based on their frequency response, which is determined by the nature of their biophysical properties. By training customized artificial intelligence models using acoustic signatures from cell lines, the system identifies oncological patterns with a reliability exceeding 90%.

The primary competitive advantage of this implementation is its time efficiency: sample processing and classification are completed in less than sixty seconds, while simultaneously eliminating the need for additional resources or infrastructure. This technology not only represents an advance in the development of advanced national technologies applied to medical instrumentation and signal processing, but also offers a scalable and low-cost solution for the oncology and materials characterization industry. The proposal aligns with goals to improve healthcare infrastructure, transforming artificial intelligence research into practical solutions with significant social impact.

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NON-DESTRUCTIVE TESTING OF PLASMA-ENHANCED GRAPHENE COATINGS ON TI-6AL-4V

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In this study, the Plasma Enhanced Chemical Vapor Deposition (PECVD) process was used to create graphene coatings on substrates of an ELI grade Ti-6Al-4V alloy. Enhancing the material surface characteristics was the aim of this investigation [1]. Non-destructive methods including Raman Spectroscopy, Thermoelectric Potential and Eddy Currents were used to characterize the material. All samples—coated and uncoated—were subjected to some surface roughness measures. A mixture of hydrogen and methane gases with an equimolar feed ratio (1:1 H_2:CH_4) at 850°C and a plasma exposure of 150 Watts for 15 minutes was used as the precursor to create graphene micro-structured coatings.

The presence of homogeneous micrometric graphene on the surface of Ti substrates was confirmed by Raman spectroscopy. Absolute thermoelectric potentials between 1.9 and 3.4 µV/K were shown by graphene coated Ti-6Al-4V ELI substrates, suggesting metallic-like behavior and applicability for thermoelectric sensing. Phase angle and substrate thickness were found to be inversely correlated, while computed electrical conductivity was shown to be directly correlated. Surface roughness increased slightly following graphene deposition, but values were still similar to those of the base alloy, maintaining compatibility for biomedical integration. SEM analysis of the graphene coating's thickness revealed that the PECVD deposited films are roughly 1 micron thick. These findings lend credence to possible uses in energy harvesting devices, wearable or implanted temperature sensors, and intelligent biomedical interfaces [2].

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NON-DESTRUCTIVE TESTING OF PLASMA-ENHANCED GRAPHENE COATINGS ON TI-6AL-4V

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DETERMINATION OF ELASTIC MODULUS IN RECYCLED-GLASS AGGREGATE CONCRETE BY ULTRASONIC MEANS

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Non-destructive testing (NDT) methods have become essential tools in the modern construction and materials industries. Among them, ultrasonic pulse velocity (UPV) method stands out due to their precision, versatility, and ability to assess the internal condition of materials without causing damage [1]. Ultrasonic method is widely used for detecting cracks, voids, and heterogeneities, as well as for estimating mechanical properties such as stiffness and compressive strength. The ultrasonic method is particularly valuable for evaluating the durability and integrity of concrete structures, where traditional destructive tests can be costly or impractical for in-service elements. In general, the ultrasonic method can be configured in different transmission arrangements such as the pulse–echo and emission- transmission techniques, each of them influencing the accuracy and energy of the received pulse. This study presents an integrated experimental evaluation of recycled-glass aggregate concrete (RGAC) through both non-destructive ultrasonic and destructive mechanical testing. Ultrasonic pulse velocity measurements were performed using the pulse–echo and emission-transmission ultrasonic techniques to determine the dynamic modulus of elasticity, while static compression tests in accordance with ASTM C469 were used to obtain the static modulus. The ultrasonic setup employed transducers operating at 500kHz and 100 kHz with a fixed path length of 5 cm. Experimental results revealed dynamic modulus values ranging from 32 to 51 GPa and static moduli between 17 and 41 GPa, depending on the recycled-glass content. The statistical analysis indicated a good linear correlation between dynamic parameters and compressive strength ($R^2 \approx 0.80$), whereas the static modulus exhibited a stronger correlation ($R^2 \approx 0.90$). Density was also measured to analyze its influence on ultrasonic velocity and stiffness parameters.

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Effect of SiO_2 Particle Morphology on the Retention of Rhodamine B from Contaminated Water

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Industrial effluents from the textile, paper, plastic, cosmetic, and pharmaceutical sectors constitute one of the main sources of contamination of aquifers due to their high dye content. Among these compounds, Rhodamine B (RhB) is one of the most widely used synthetic dyes and has been reported to cause adverse effects on both the marine ecosystem and human health [1,2]. However, conventional wastewater treatment methods often show limited efficiency in removing this type of pollutant, motivating the search for more efficient alternatives [3].

The aim of this study was to evaluate the effect of SiO_2 nanoparticle structure (solid and porous) on RhB retention capacity. The materials were synthesized via the Stöber method, using an alkoxysilane precursor (TEOS); in the case of porous nanoparticles, a cationic surfactant (CTAB) was additionally incorporated to induce pore formation. The resulting materials were characterized by ultraviolet-visible (UV-Vis) and Fourier-transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM), in order to analyze their chemical, morphological, and structural properties.

The RhB retention capacity was evaluated in a contaminated water matrix. UV-Vis results showed that only the porous SiO_2 nanoparticles retained the dye, evidenced by the appearance of a characteristic absorption band around 540 nm after contact with the RhB solution, whereas the solid SiO_2 particles showed no signal. The interaction between the dye and the nanoparticles was further confirmed by FT-IR, through the appearance of new vibrational bands associated with the $O-H$ and $C=O$ stretching of the carboxylic acid ($3200\ cm^{-1}$ and $1700\ cm^{-1}$), $C-H$ stretching of the amine ($2930\ cm^{-1}$), $C=C$ aromatic ring stretching bands ($1560-1650\ cm^{-1}$), and $C-O-C$ stretching ($1140\ cm^{-1}$). Quantitatively, the porous nanoparticles achieved a retention capacity of up to 65%, demonstrating their potential as adsorbents for the removal of synthetic dyes.

Taken together, these results suggest that porous SiO_2 nanoparticles constitute a promising alternative for the retention and detection of Rhodamine B, and establish a basis for their future application in other matrices of interest, such as water, cosmetics, drugs, and food.

Keywords: dyes, wastewater, porous materials, SiO_2, Rhodamine B, UV-Vis, FT-IR, retention

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Polymat Contributions

CHARACTERIZATION AND IN VITRO EVALUATION OF CHITOSAN/GUM ROSIN COATINGS ON *ESCHERICHIA COLI*

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In this study, coatings from chitosan, gum rosin and calcium oxide (CaO) microparticles synthesized from *Moringa oleifera* Lam. extract were characterized and their antimicrobial activity (colony forming units, CFU) against *Escherichia coli* was evaluated. The microparticles were characterized by transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDS), and dynamic light scattering (DLS) to determine their morphology, composition, and size distribution. From Fourier transform infrared spectroscopy (FTIR) the functional groups were identified. TEM analysis revealed spherical microparticles. EDS analysis confirmed the presence of oxygen (83.4%) and calcium (16.6%). DLS analysis indicated a particle size range between 246.1-284.1 nm. The coating formulations included chitosan (1 %), gum rosin (1 %, 2 %, and 3 %) and the CaO microparticles. The antimicrobial activity was evaluated at 24 and 48 h. The results showed that the coatings exhibited inhibitory effect on *E. coli* with a decrease in bacterial growth compared to the control (only chitosan). After 24 h, the formulations containing 2 % of gum rosin and the microparticles exhibited complete inhibition. After 48 h, the formulation with 3 % of gum rosin showed the lowest bacterial count (4.5 ± 1.29 CFU). The results suggests the potential of combining natural products and biodegradable materials as a future alternative for the elaboration of functional coatings to reduce *E. coli* on horticultural products.

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Chitosan Based Nanofibers in Strawberry Seed Germination

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The increase in CO2 emissions over the last decade, due to food waste, has driven the development of sustainable agriculture. Strawberries (Fragaria × ananassa) are highly perishable fruit, especially during germination, due to low germination rates, long development times, and pathogenic threats such as grey mould; this results in the waste of valuable economic, energetic and enviromental resources. This work focuses on the search for sustainable alternatives of fungicides with the optimization of resources to reduce waste during strawberry seed germination. In the greenhouse, optimal energetic conditions were defined to improve germination rate, resulting in more effective and earlier germinations. Besides, chitosan is proposed as a biodegradable, biocompatible, and antifungal material, as an alternative to conventional fungicides that cause significant environmental pollution. Fibers of 13 µm and 103 µm in thickness were obtained as a sustainable strategy to inhibit fungal proliferation during strawberry seed germination. Nanofibers were obtained from a chitosan-polycaprolactone (PCL) solution using a homemade electrospinning system. The chitosan was dissolved in a mixture of organic acids, with constant agitation, and tempeture control. The obtained nanofibres were used with straberry seeds, in a seed starter kit, under controlled conditions to obtain a fungus free germination.

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USE OF INNOVATIVE AND SUSTAINABLE TECHNOLOGIES FOR THE PRESERVATION AND HANDLING OF BIOLOGICAL SYSTEMS IN THE MINING INDUSTRY

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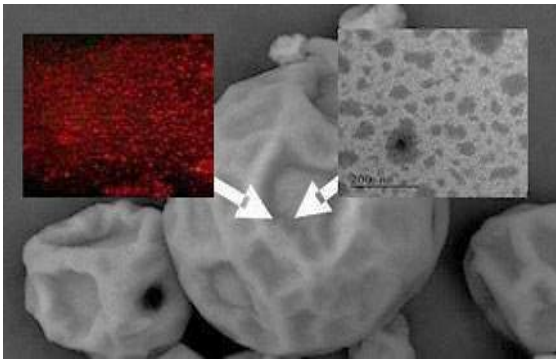
Biometallurgical processes offer promising alternatives for metal recovery and the bioremediation of environments affected by mining activities. However, the industrial implementation of these technologies remains limited, primarily due to two factors: the high costs associated with monitoring metabolic activity and the genetic stability of bacteria during prolonged operation [1]. Currently, it is estimated that, worldwide, only 5% of the gold and 20% of the mined copper are obtained through biomining processes, highlighting the need to develop strategies that promote the conservation and availability of microorganisms of interest [2].



In this context, microencapsulation is a promising strategy for facilitating the handling and preservation of these microorganisms. In this study, *Acidithiobacillus thiooxidans* was encapsulated via spray drying, using various biopolymers as wall materials. The resulting microcapsules exhibited physicochemical properties suitable for storage, with water activity (aw) below 0.55 and moisture content under 10%. Scanning electron microscopy analysis revealed spherical, homogeneous microparticles with no evidence of structural collapse, suggesting adequate mechanical stability. Furthermore, a bacterial survival rate of 1.4 × 10^9 cells/mL and a leaching capacity of 95% were achieved. Notably, the encapsulated bacteria remained viable for over two years, ensuring their storage and availability for long-term biohydrometallurgical applications. These results demonstrate that spray-drying microencapsulation is an efficient, scalable, and sustainable technology for preserving industrially relevant microorganisms, particularly by contributing to the development of more robust and environmentally responsible biometallurgical processes.

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ADVANCED OXIDATION TECHNOLOGIES: $CoFe_2O_4$ AS A CASE STUDY FOR SUSTAINABLE WATER REMEDATION

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The continuous discharge of emerging contaminants into aquatic ecosystems poses enormous challenge to both environmental science and the wastewater treatment industry. Pharmaceuticals like diclofenac are routinely detected in secondary effluents and natural water[1]. Consequently, developing efficient, sustainable advanced oxidation technologies (AOTs) that achieve high degradation efficiencies while minimizing energy consumption and operational costs is a priority. Among AOTs, photocatalysis, sonocatalysis, and sonophotocatalysis have emerged as promising strategies, as each activation pathway generates reactive oxygen species (ROS) through distinct physicochemical mechanisms[2][3]. This work presents a rationally designed $CoFe_2O_4$ spinel ferrite synthesized via a modified Pechini route and a study systematically investigates how distinct activation regimes—ultraviolet, visible light, ultrasound, and their coupled sonophotocatalytic combinations—govern catalytic performance during diclofenac degradation. Particular focus is directed toward elucidating how each excitation route modulates ROS production mechanisms and degradation kinetics. Ultimately, this comprehensive evaluation provides actionable guidelines for selecting optimal activation strategies based on operational demands, demonstrating how defect-engineered nanostructures can advance scalable, energy-efficient AOTs for sustainable water remediation.

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FUNCTIONAL SUPERPARAMAGNETIC NANOSTRUCTURES ORIENTED TO DRUG DELIVERY

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Superparamagnetic Nanoparticles (<20 nm) were encapsulated with *Mentha Arvensis* extracts as second metabolite to add hydroxyl (-OH) bonding over their surface. These can improve their cell viability for therapeutic and drug release applications [1]. *Mint* plant is known for its richness in flavonoids; however, there is no study that integrates its use in Zn-Ferrite nanoparticles coating. This study reports the green synthesis and functionalization of Zn-Ferrite nanoparticles coated with *Mentha Arvensis* ($Zn_{0.1}Fe_{2.9}O_4@Polyphenols$) by co-precipitation method. Preliminary results obtained by X-Ray Diffraction have showed: inverse spinel structure with *d*= 16.05 nm, *a*= 8.3957 Å, FCC No. PDF 96-900-6895. Transmission Electron Microscopy (TEM) characterization revealed quasi-spherical crystalline structures with d~17 nm and *Mentha Arvensis* thickness ~20 nm. X-ray photoelectron spectroscopy (XPS) showed elemental chemical composition as $Zn_{0.063}Fe_{2.937}O_4$ and oxidation states spectra of O1*s*, C1*s*, Zn2*p*, and Fe2*p* bonds. Topographic images and Magnetic Force Microscopy (MFM) showed single magnetic domains with uniaxial magnetic field flux. The observed structure, composition, and surface properties confirm the coated of the nanoparticles by phenolic groups, for future formulations in the application of drug release.

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NUMERICAL ANALYSIS OF THE EFFECT OF CASTING SPEED AND SEN IMMERSION DEPTH ON FLUID DYNAMICS IN A CONTINUOUS CASTING SLAB MOLD

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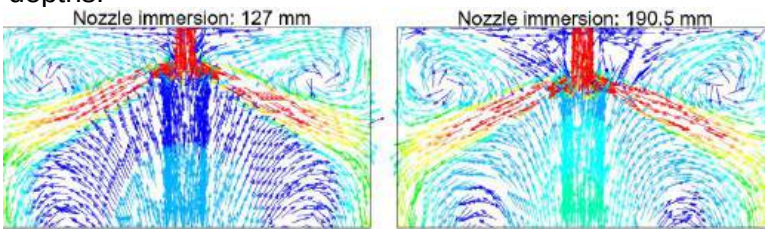
One of the fundamental challenges in the metallurgical industry is increasing productivity without sacrificing the quality of the steel produced [1-2]. One common strategy to achieve this is to increase the casting speed while ensuring flow stability for both submerged entry nozzle (SEN) immersion depths within the continuous casting mold [3-4]. Based on this, the present study numerically evaluated the fluid dynamic effects of increasing the casting speed from 1.1 to 1.3 and 1.5 m/min using two SEN immersion depths of 127 and 190.5 mm on the behavior of the molten steel within the SEN and the mold. A three-dimensional model based on the Navier–Stokes equations, the standard k–ε turbulence model and the Volume of Fluid (VOF) method was employed, taking into account the phases of steel, air and slag. The results showed that increasing the casting speed led to an increase in flow velocity within the SEN of 18.14% and 36.30% compared to the lowest casting speed. Additionally, the free-surface velocity increased by 18.27% and 38.97% for an immersion depth of 127 mm and by 17.04% and 32.35% for an immersion depth of 190.5 mm. Within the mold, the 190.5 mm immersion depth generated jets that impinged on the narrow faces with greater penetration depth and velocity. Comparing the two immersion depths, the shallower immersion produced the highest free-surface velocities, exceeding those obtained with the deeper immersion by up to 47.87%. Despite these increases in free-surface velocity, the maximum velocity remained below the critical value associated with slag-layer instability. This indicates that the SEN design performs adequately as the casting speed increases for both immersion depths.



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Nanoalambres de ZnO: Crecimiento y Aplicaciones

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Los nanoalambres semiconductores representan una plataforma prometedora para el desarrollo de tecnologías innovadoras en el sector de la salud, gracias a su alta relación superficie-volumen, sus propiedades electrónicas ajustables y su facilidad de funcionalización superficial. En esta charla se presentarán avances recientes en el diseño y la síntesis de nanoalambres de óxidos metálicos, en particular de ZnO, con enfoque en aplicaciones biomédicas. Se discutirá su uso como plataformas multifuncionales para la detección y el tratamiento de bacterias resistentes a antibióticos, destacando los mecanismos fisicoquímicos involucrados, como la generación de especies reactivas de oxígeno y la interacción entre la superficie y el patógeno. Asimismo, se analizará cómo los parámetros estructurales, como el diámetro, la longitud y la formación de heteroestructuras, influyen en la sensibilidad, la selectividad y la biocompatibilidad de los dispositivos. Finalmente, se abordarán las perspectivas para el desarrollo de nanosistemas inteligentes capaces de integrar diagnóstico y acción terapéutica, contribuyendo al combate de la resistencia antimicrobiana y al avance de la nanomedicina.

Keywords: E. coli, Biodetection, AMR bacteria

A comparative study of the structural, optical, and electrical properties of indium- and gallium-doped MgxZn1−xO films for TCO applications

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Two sets of $Mg_{0.10}Zn_{0.90}O$ thin film samples, doped with Ga or In donor impurities and prepared using spray pyrolysis, were examined. The study focuses on comparing how residual stress influences the initiation of the self-compensation process and the defects that arise at high donor doping levels. This doping approach is important for potential and future applications of $Mg_{0.10}Zn_{0.90}O$ thin films as transparent conducting oxides, particularly in optoelectronic devices. The films were doped with gallium or indium at concentrations ranging from 0% to 4.0 at.%. Deposition was performed at a constant temperature of 350°C, followed by heat treatment at 350°C under a nitrogen atmosphere. The characterization techniques used included scanning electron microscopy, X-ray diffraction, energy-dispersive X-ray spectroscopy, optical transmittance and absorption measurements, and electrical resistivity assessments. Residual stress in the films was evaluated by accounting for the differences in ionic radii of the dopants, smaller for gallium and larger for indium compared to Zinc and magnesium. The morphological, structural, optical, and electrical properties of the thin films were analyzed and compared, considering the effect of stress at different doping levels on the onset of the self-compensation process.

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Structure, composition, optical and electrical properties of In-doped $Mg_{0.10}Zn_{0.90}O$:2%Al films for transparent conductive oxide applications

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The effect of indium doping on $Mg_{0.10}Zn_{0.90}O$:2%Al films were examined by analyzing their morphology, chemical composition, crystal structure, optical transmittance, and electrical properties. The $Mg_{0.10}Zn_{0.90}O$:2%Al thin films were prepared using the spray pyrolysis method at a fixed deposition temperature of 400°C. The concentration of the Indium donor element varies from 0.0 to 3.5 at% with the step of 0.5 at%, while the concentration of the second Al donor remains constant at 2 at%. The obtained films were characterized using the following experimental techniques: scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), optical transmittance measurement, and the electrical resistivity was monitored as well.
Residual stress in the films was estimated based on the XRD analysis in dependence on the variation of Indium content. In addition, the effects of residual stress on the initiation of the self-compensation process in the films were analyzed. The $Mg_{0.10}Zn_{0.90}O$:2%Al thin films are interesting as transparent conducting oxides (TCOs) for ZnO-based optoelectronic devices.

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Abstract preparation

DEVELOPMENT AND CHARACTERIZATION OF INNOVATIVE INHIBITORS FOR THE PROTECTION OF API 5L X70 STEEL IN DIFFERENT CORROSIVE MEDIA

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Corrosion in metallic pipelines represents a major challenge in industrial sectors such as oil and gas, particularly under aggressive environments where the presence of moisture, salts, and dissolved gases accelerates degradation processes[1]. In this study, innovative corrosion inhibitors were developed and characterized to enhance the protection of pipeline materials. The synthesized compounds were evaluated using electrochemical techniques, including electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization, to determine their inhibition efficiency and adsorption behavior on metal surfaces. Surface characterization analyses were also performed to elucidate the interaction mechanisms between the inhibitors and the substrate. The results demonstrate that the proposed inhibitors significantly reduce corrosion rates by forming a protective film on the metal surface, with efficiency depending on concentration and environmental conditions. The findings provide valuable insights into the design of advanced corrosion inhibitors and their potential application in extending the service life of pipeline systems.

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Processing of the Mezcal Bagasse Lignocellulosic Matrix via Heterogeneous Catalytic Systems for Industrial Bioethanol Production

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The diversification of the industrial energy matrix requires the development and utilization of new sustainable raw materials. This work approaches Agave potatorum bagasse, a byproduct of the mezcal industry, as a strategic lignocellulosic material for the synthesis of second-generation bioethanol. From a materials science perspective, the main challenge lies in the efficient depolymerization of its complex solid structure (composed of cellulose, hemicellulose, and lignin). To overcome this, structural modification routes driven by heterogeneous catalytic systems were evaluated: a chemical treatment acting on the solid phase using an inorganic catalyst (98% concentrated H_2SO_4 in a 2.5% solution) to fracture the matrix and release short-chain sugars, a selective enzymatic biocatalyst aimed at breaking glycosidic bonds, and a combined catalytic scheme. The structural modifications of the material were monitored using thermogravimetric analysis (TGA) and FTIR spectroscopy. The highest conversion yield was obtained through combined hydrolysis on a material conditioned to a #30 sieve particle size, achieving an 8% alcohol concentration after fermentation and double distillation. These results demonstrate that the application of specific catalytic materials in heterogeneous solid-liquid interfaces allows for the molecular-level modification of agro-industrial residues, converting them into viable and scalable substrates for the energy industry.

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X-RAY SOLUTIONS FOR ADVANCED MATERIALS CHARACTERIZATION

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Abstract

To address the increasing analytical demands in materials science and industrial research, advanced X-ray spectrometry and diffraction solutions developed by Bruker are presented for the comprehensive characterization of complex material structures. The methodology encompasses an integrated analytical profile focusing on multi-element quantification and phase identification across solid, powder, and thin-film matrices [2, 3]. By combining high-stability X-ray optics, advanced generators, and next-generation detectors, these systems enable non-destructive evaluation of elemental composition, crystallographic phases, residual stress, and microstructure without altering sample integrity [2]. Key application profiles include quality control in alloys and ceramics, catalyst monitoring in environmental processes, and strict regulatory compliance testing in technological polymers and coatings [3]. Overall, these technological platforms provide high precision, outstanding operational repeatability, and superior throughput for synthesis optimization and failure diagnosis at pilot and industrial scales [1, 2].

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MATERIAL CHARACTERIZATION BY MEANS OF EDX-7200 X-RAY FLUORESCENCE

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Abstract

To meet the increasing demand for rapid and non-destructive elemental testing in both industrial and research environments, an applied materials characterization profile was developed using Energy Dispersive X-Ray Fluorescence (EDXRF) spectrometry with the Shimadzu EDX-7200 system [1]. This analytical protocol focused on multi-element quantification from sodium ($_{11}$Na) to uranium ($_{92}$U) under controlled vacuum, helium, and air atmospheres, maximizing sensitivity across diverse matrices [2]. Key application profiles included alloy grade verification, thickness measurement of thin films and coatings, environmental regulatory compliance (RoHS/WEEE) in polymers, quality control in ceramics, and the quantitative determination of spent catalysts and filter media used in environmental processes [3]. By incorporating a high-resolution silicon drift detector (SDD) and accommodating solid, liquid, and powder samples, the setup enabled precise trace and impurity detection without modifying the physical structure of the materials [1]. Overall, this approach highlights the analytical versatility of EDXRF for synthesis optimization, manufacturing quality control, and failure diagnosis at pilot and industrial scales [2, 3].

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One energy: Hydrogen production via catalytic aqueous reforming of biomass.

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The continuous increase in pollutant emissions, the rise in energy consumption and development of new technologies have led to a worrying climate outlook. This context demands the diversification of the energy mix and the exploitation of renewable energy sources to mitigate the environmental impact of anthropogenic activities [1]. Hydrogen has emerged as a promising solution due to its enormous potential for applications in electricity, transportation, and industry, with an almost total reduction in greenhouse gas emissions. However, its production and storage remain a challenge. In general, current hydrogen production methods require high temperatures and/or pressures, as is the case with reforming, pyrolysis, thermolysis, etc. [2]. An alternative to overcome this problem is the transformation of platform molecules from biomass into hydrogen like glycerol, residue from biodiesel production has become an opportunity with significant potential due to its high hydrogen content [3]. One energy seeks to modify the conventional reforming process and use a heterogeneous catalyst to reduce the extreme conditions of conventional processes developing a tailor-made reactor. Also, the modify of process allow reduce the emissions pollutant and increase process selectivity for drive the growth of hydrogen technology.

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Structure–Property Relationships in Iodine Capture and Fluorescence Sensing by SU-101 and SU-102 Ellagate Metal–Organic Frameworks

Celene García-Carvajal[1], Juan P. Arismendi,[1] Catalina Biglione,[2] Isaí U. Alva-Sandoval,[1] Marco L. Martínez,[1] José Luis Belmonte-Vázquez,[3] Diego Solis-Ibarra,[1] Patricia Horcajada,[2]* Ilich A. Ibarra[1]* and Yoarhy A. Amador-Sánchez,[1]*

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Developing multifunctional porous materials that combine iodine capture and optical sensing using accessible and renewable building blocks is attractive for practical applications [1]. Here, we compare SU-101 and SU-102, two robust metal–organic frameworks constructed from commercially available, plant-derived ellagic acid, featuring Bi(III) and Zr(IV) metal nodes, respectively [2,3]. Their distinct local coordination environments and framework architectures provide a platform to examine how the framework microenvironment controls iodine uptake and fluorescence transduction. Under identical iodine-vapor exposure conditions, SU-101 and SU-102 reached experimental loadings of approximately 331 and 1008 mg g^{-1}, respectively, while EDS independently confirmed iodine incorporation and supported the higher loading observed for SU-102. PXRD and FTIR showed substantial preservation of framework integrity after iodine uptake. Solid-state UV–visible and photoluminescence measurements revealed iodine-induced visible absorption and structure-dependent fluorescence quenching. Time-resolved photoluminescence showed that this quenching was not accompanied by lifetime shortening, indicating a substantial static contribution to the optical response [4]. Quantitative fluorescence titrations in cyclohexane yielded detection limits of 107.1 µM for SU-101 and 2.8 µM for SU-102. Thus, although SU-102 adsorbs only about three times more iodine than SU-101, its detection limit is approximately 39 times lower, demonstrating that iodine capture and optical transduction are related but non-proportional properties governed by the framework microenvironment.

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NANOMETRIC THIN FILMS OF $MAPb_{0.9}Sn_{0.1}I_3$ PROCESSED WITHOUT INERT ATMOSPHERE, ADDITIVES OR AUXILIARY TECHNIQUES

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This work present the synthesis of mixed-perovskite thin films under standard atmospheric conditions, without additives or stabilizers. The precursor solutions were prepared using mehtylammonium iodide (MAI), lead iodide (PbI_2), and tin chloride ($SnCl_2$) dissolved in dimethyl sulfoxide (DMSO) and dimethylformamie (DMF). A molar ratio of 1:0.9:0.1:1 was used for MAI, PbI_2, $SnCl_2$, and DMSO, respectivelym dissolved in 600 μL of DMF.

Deposition was carried out in a single step using the spin-coating technique, with parameters set to 5000 rpm for 20 seconds. During deposition, the use of ethyl acetate as an anti-solvent was optimized by varying the volume from 140 to 300 mL. The films underwent heat treatment at 100 °C, with durations varying between 2, 5, 10, 20, 30, and 60 minutes.

The resulting films were characterized via UV-Vis spectroscopy to determine their absorance, transmittance, and relectance. Profilometry was also used to measure film thickness and surface roughness.

The results shown in this research, demonstrate the feasibility of synthesizing tin-containing perovskite films, less lead, without controlled atmosphere. This procedure colud be used in the future solar cell industry to produce active layers for photovoltaci cells.

Acknowledgements

The authors gratefully acknowledge the UNAM projects and the Secretaría de Ciencia, Humanidades, Tecnología e Innovación (SECIHTI) for doctoral scholarship and financial support. The authors also acknowledge the use of the laboratory facilities at IER-UNAM and University of Sonora.

From Laboratory Research to Industrial Applications: Multifunctional Nanomaterials for Water Treatment and Remediation

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The treatment of wastewater generated by textile, pharmaceutical, chemical, and food-processing industries represents one of the major environmental and technological challenges worldwide. The presence of dyes, persistent organic compounds, oils, and emerging contaminants requires the development of advanced materials capable of improving the efficiency and sustainability of conventional treatment technologies. In this context, multifunctional nanomaterials have emerged as promising alternatives due to their tunable physicochemical properties, high surface area, and enhanced catalytic performance [1].

This presentation describes several research lines focused on the design, synthesis, characterization, and evaluation of functional nanomaterials for water treatment and remediation applications. Materials based on titanium dioxide (TiO_2), TiO_2–MoS_2 hybrid systems, and TiO_2–Ag nanocomposites are presented as photocatalytic platforms for the degradation of dyes, organic pollutants, and emerging contaminants of industrial relevance. Strategies to optimize their structural, optical, and surface properties are discussed in order to improve catalytic efficiency, stability, and operational performance.[2]

Advanced characterization techniques, including spectroscopic, structural, and morphological analyses, are employed to establish correlations between material properties and functional behavior. The obtained results demonstrate the potential of these nanomaterials for integration into sustainable water-treatment technologies and environmental remediation processes [2].

Finally, perspectives on scaling-up, implementation in continuous-flow photocatalytic reactors, and potential industrial deployment are presented, highlighting their contribution to the development of innovative technologies for sustainable water-resource management and environmental impact reduction.

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STRUCTURE–PROPERTY RELATIONSHIPS AND PESTICIDE UPTAKE IN κ-CARRAGEENAN/CHITOSAN/PVA HYDROGEL MEMBRANES

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Hybrid hydrogel membranes based on κ-carrageenan (κ-CRG), chitosan (CS) and poly(vinyl alcohol) (PVA) were prepared by solvent casting over a wide range of κ-CRG:CS/PVA volume ratios (1:9 to 9:1). The influence of composition on membrane structure, physicochemical properties and polyelectrolyte complex (PEC) formation was systematically investigated to elucidate composition-network organization-property relationships. Additionally, preliminary adsorption assays were carried out using diazinon, paraquat and 2,4-D as model pesticide contaminants because of their environmental relevance and occurrence in aquatic systems in Mexico and worldwide [1, 2]. FT-IR analysis supported hydrogen bonding among polymer chains and electrostatic interactions between the sulfate groups of κ-CRG and protonated amino groups of CS, while morphological analysis revealed composition-dependent heterogeneous fibrillar features consistent with PEC-rich domains. These composition-induced structural changes were accompanied by variations in crystallinity, surface roughness, wettability, water uptake, and mechanical response under hydrated conditions. Pesticide uptake was dependent on both membrane composition and contaminant identity. Among the evaluated formulations, the 9:1 membrane exhibited comparatively low equilibrium swelling (111.0 ± 10.8%), a high elastic modulus (8.01 ± 0.96 MPa), and the highest diazinon adsorption capacity (3.49 ± 0.47 mg/g). In contrast, the 7:3 formulation showed the highest adsorption capacity for 2,4-D (4.25 ± 0.47 mg/g). For paraquat, all formulations exhibited low overall retention, characterized by rapid initial uptake followed by subsequent desorption, indicating comparatively weak or reversible interactions with the polymer network. These findings demonstrate that κ-CRG/CS/PVA membranes can be rationally tuned through composition-induced PEC formation, providing a composition-network organization-property framework that links network structure and bulk properties with contaminant-specific uptake and retention. This framework provides a basis for the rational optimization of functional hybrid hydrogels for water remediation and other applications requiring composition-dependent control of their physicochemical properties.

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REVALORIZATION OF BREWING MALT RESIDUE FOR OBTAINING BIOETHANOL AS A FUEL ADDITIVE

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The valorization of agro-industrial waste constitutes an alternative for diversifying the sources of raw materials intended for biofuel production [1].This study evaluated the revalorization of brewer's spent grain (BSG) for obtaining bioethanol with potential use as an oxygenating additive in fuels.

The experimental process included the thermogravimetric characterization of the material, which determined a volatile matter content of 71.92%, as well as starch, hemicellulose, and cellulose contents of 10.43, 35.93, and 9.69%, respectively. From the thermal analysis, a maximum pretreatment temperature of 131.02 °C was established. Acid hydrolysis was evaluated using H_2SO_4 and HCl at different concentrations and reaction times [2], obtaining a maximum soluble solids concentration of 13 °Brix using 4% HCl for 120 min. Subsequently, enzymatic hydrolysis was carried out using glucoamylase at a pH of 5.4–5.6 and a temperature of 50–60 °C for 1 h. The resulting hydrolysates were subjected to fermentation with *Saccharomyces cerevisiae* and subsequently to a distillation process.

Characterization of the distillates by FTIR spectroscopy and gas chromatography confirmed the presence of ethanol [3]. An alcohol concentration of 71% was achieved, with a water content of 29%, a density of 0.9744 g/cm³, and a pH of 6.0. These results demonstrate the obtainment of ethanol from brewer's spent grain; however, the product did not meet the established specifications for anhydrous bioethanol, mainly due to its water content [4].Consequently, the need to incorporate improvements in the distillation process to increase product purity and evaluate its potential as an oxygenating additive in fuels is identified as a replacement for MTBE [5] [6].

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EFFECT OF RADIATION AND TEMPERATURE ON CULTIVATION FILMS IN CONTACT WITH A SULFUR-BASED FUMIGANT

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It is currently known that lifespan of agricultural mulch films can vary, ranging from a limited duration to as long as three years, depending on factors such as manufacturing quality, materials, additives, and design, as well as usage methods and exposure conditions. This study aimed to assess the durability of mulch films exposed to field conditions involving the use of sulfur-based agrochemicals. Based on specifications from LyondellBasell industry, the study compared three different films, each one incorporating a specific protective agent designed to resist weathering. Field conditions, including climatic factors (rainfall, solar radiation, wind, and temperature) and the application of agrochemicals (fumigants, fertilizers, pesticides, and herbicides), were monitored over a one-year period. Subsequently, the films integrity was evaluated using atomic force microscopy (AFM) and mechanical property testing. Additionally, a controlled laboratory study was carried out to observe the stability of each film against chemical attack by vapors from the sulfur-based fumigant dimethyl disulfide (DMDS), while eliminating variables such as fluctuations in light, temperature, humidity, and radiation present in the experimental field. The results indicated that DMDS vapor alters the films plasticity characteristics over time, both with and without weathering exposure. AFM imaging revealed visible areas of alteration in all films treated with DMDS (Figure 1).

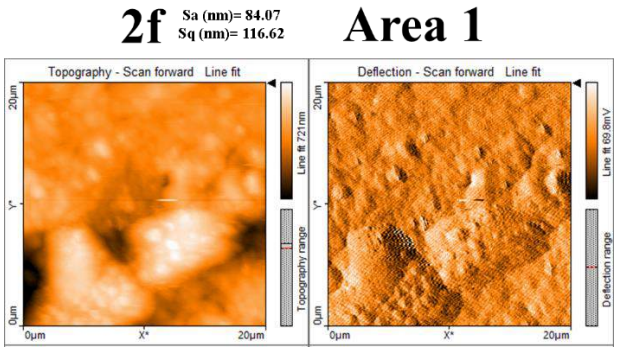

Figure 1. AFM topography of the 2F film.

Characterization of an ER5356 aluminum alloy wall fabricated using RMD metal transfer mode

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Wire arc additive manufacturing (WAAM) is distinguished as the directed energy deposition (DED) process with the best buy-to-fly ratio, high deposition rates, and the ability to manufacture large-scale components [1]. Aluminum alloys of the 5000 series contain Mg levels that typically do not exceed 10.5% by weight, providing good ductility, toughness, and corrosion resistance, as well as high mechanical strength, low cost, and low density; these properties have led to their extensive use in automotive, aerospace, naval, and aeronautical applications [2]. WAAM technology commonly uses the GMAW process for material deposition. There are advanced variants of the filler metal transfer modes that reduce the heat input (HI) and the amount of spatter during deposition; one of these is the Regulated Metal Deposition (RMD) transfer mode [3]. The use of RMD in additive manufacturing applications of non-ferrous alloys has been rarely studied; therefore, it is necessary to conduct a further study of this technology and assess the feasibility of its application.

In this study, a 54 layer wall was fabricated using the ER5356 alloy. An average height of 10.5 cm was achieved using a semi-automated system. During the deposition process, a stable metal transfer rate was achieved, with an average HI of 0.032 kJ/mm. The deposited mass was quantified, and, with the aid of a 3D scan, the effective mass was calculated, resulting in a buy-to-fly ratio of 2.8. Subsequently, a macroscopic analysis of the observed defects was conducted to determine their root cause. Finally, a specimen was extracted for macrographic and metallographic analysis to report the presence and size of internal defects and microstructural changes in the build-up direction, respectively. The results obtained were correlated with the microhardness levels at the lower, middle, and upper sections of the specimen; no significant change was detected, and an average hardness of 87.63 ± 8.8 HV was reported.

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Sargassum-Derived Nanocellulose as a Sustainable Biopolymer Matrix for Magnetically-Enhanced Electrochemical Sensors

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The presence of emerging contaminants in water systems poses a severe environmental and public health threat, demanding the development of rapid, highly sensitive detection platforms. Concurrently, the valorization of abundant biomass offers a sustainable pathway for the synthesis of advanced materials. This work presents the development of a magnetic nanocomposite based on nanocellulose extracted from Sargassum biomass using a green deep eutectic solvent (DES) system composed of choline chloride and oxalic acid. Operating within an eco-friendly framework, the extracted nanocellulose serves as a supportive matrix that is saturated with magnetite. Subsequently, an in situ synthesis of nickel (Ni), gold (Au), and manganese (Mn) nanoparticles is performed to decorate the composite, significantly enhancing its overall physicochemical and catalytic properties. The nanocomposite is comprehensively evaluated through structural and chemical analyses (FTIR, Raman spectroscopy, and XRD), morphological and elemental mapping (SEM-EDS), mechanical testing (tension and compression), and magnetic assessment (VSM). For environmental applications, the composite is directly immobilized onto carbon and conductive glass electrodes, effectively bypassing the need for conventional polymeric binders such as Nafion to fabricate the modified electrodes. The electrocatalytic activity against various pollutants is evaluated using cyclic and pulse voltammetry. Additionally, a systematic study investigates the effect of external magnetic fields on the sensor's sensitivity and selectivity, leveraging the material's magnetic properties to improve detection limits. Ultimately, this approach advances the design of sustainable functional materials while aligning with the core goals of the circular economy.

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Integration of a Real-time Parameter Monitoring and Control System for Biogas Generation Systems for the Utilization of OMSW

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Anaerobic digestion (AD) facilities for the treatment of the organic fraction of municipal solid waste (OFMSW) have not been successfully developed in Mexico, despite the process providing an adequate treatment for this type of waste. Furthermore, it enables the harnessing of biogas—composed mainly of methane—preventing its release into the atmosphere, as it is a gas potentially more polluting than CO_2 [1]. One of the main difficulties is the management of organic waste and source separation, alongside the significant operational limitations faced by anaerobic digestion systems (ADS).

Various biological, chemical, and physical factors influence the efficiency of the digestion process. Specifically, the composition and quality of the substrate, which allow for adequate mass transfer during each stage of the AD process, play a fundamental role and remain a subject of study. However, their operational dynamics, efficiency, and methane production behavior remain largely unquantified [2]. Consequently, many systems fail because the process development under external factors remains unknown.

In this work, a prototype of a mesophilic ADS is evaluated, powered by solar energy. The system is self-sufficient, featuring real-time monitoring of temperature, pressure, and biogas quality parameters to ensure operational viability, safety, and efficiency.

The integration of a data acquisition card and a control system for substrate feeding homogenization at the prototype level offers a cost-effective solution with technical foundations for scalability at residential, industrial, and commercial levels, while also identifying potential areas for future research.

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CO_2 ADSORPTION ON COPPER TETRAMERIC NANOALLOYS (Cu_3M)

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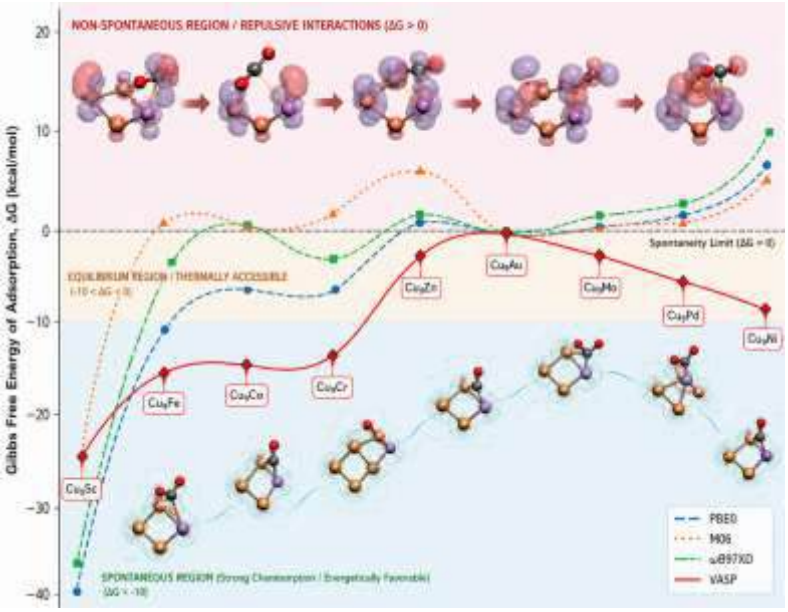

The mitigation of carbon dioxide (CO_2) emissions is one of the most urgent environmental challenges today due to its predominant role in global warming [1]. In this context, CO_2 capture and adsorption using subnanometer metallic clusters represent a promising strategy [2]. In this work, tetrameric Cu_4 and Cu_3M clusters (M = Pd, Zn, Mo, Sc, Au, Ni, Pt, Fe, Co) were optimized across various geometries and spin multiplicities using DFT calculations (PBE0/LanL2TZ) implemented in Gaussian 16. The most structurally stable isomers served as the baseline to evaluate CO_2 adsorption using the PBE0, M06, and wB97xD functionals, whose results were benchmarked against periodic calculations in VASP [3].

CO_2 adsorption onto Cu_3M clusters strongly depends on the nature of the dopant metal and the computational method employed, allowing a transition from a weak, thermolabile physisorption regime to strong, highly exergonic chemisorption. Overall, these findings demonstrate that doping effectively modulates the transition between physical and chemical interactions, thereby governing CO_2 stability on Cu_3M cluster.

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CO_2 ADSORPTION ON COPPER TETRAMERIC NANOALLOYS (Cu_3M)

Jennifer Paola Hernández-Mancera[1], Ana Leonor Acevedo Pérez[1], Francisco Nuñez Zarur[1]

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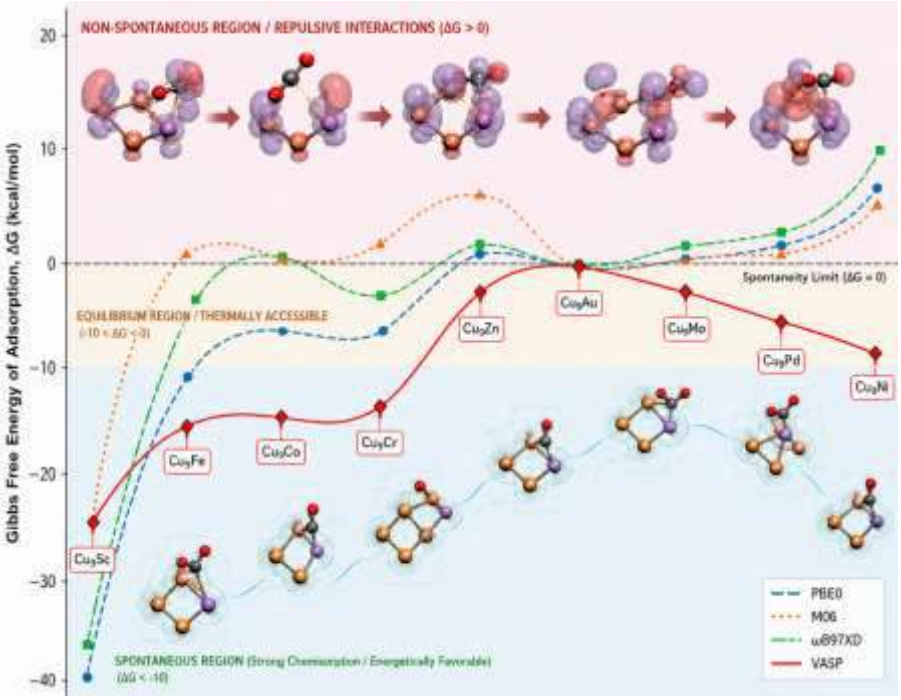

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COOLING CURVE ANALYSIS AND ESTIMATION OF THE HEAT TRANSFER BOUNDARY CONDITION DURING RAPID COOLING WITH A QUENCH RING: A COLLABORATION BETWEEN UNAM AND QUAKER HOUGHTON

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Characterization of heat extraction and metallurgical response during quenching of metallic parts is a key component in process design. There are two methodologies commonly used to accomplish it: cooling power and hardening power [1]. Cooling curve analysis is a widely-used methodology to characterize cooling power of quenching media [2], whereas the Jominy end-quench test [3] is applied to characterize the hardening power through the hardenability of steels. There are plenty of papers published on cooling curve analysis to study quench media under immersion quenching conditions; however, this information is not readily available for quench rings, which is the preferred equipment used for induction quenching.

The Universidad Nacional Autónoma de México (UNAM) and Quaker Houghton (a company that commercializes, among many other fluids, quenching media) have been collaborating to carry out cooling curve analysis during quenching of probes using aqueous polymer solutions with quench rings designed *ad hoc*. The results of this collaboration have allowed establishing the effect of: 1) quench ring design, 2) polymer concentration, 3) quenchant temperature, 4) polymer type, and 5) position of measurement of the cooling curve, on cooling power and heat extraction of aqueous polymer solutions. Five undergraduate thesis, a paper published at an international conference, and an award won by one undergraduate student at another international conference have resulted from the studies carried out at UNAM while Quaker Houghton has gained valuable knowledge on this particular quench medium. It can be concluded that this collaboration has been a win-win both for the university and the industry partner.

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Abstract preparation

KEITHLEY: Electrical Characterization for materials using wave tracers

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This seminar will present the use of a curve tracer system for the electrical characterization of materials and devices. Its architecture, operating principle, and capabilities, specifically the ability to supply voltage or current while simultaneously measuring the resulting electrical variables with high precision will be described. Through practical examples, various configurations and measurement methodologies will be demonstrated for determining resistivity and conductivity, as well as for obtaining and analyzing the characteristic curves of diodes, transistors, and solar cells. The goal is to provide a comprehensive overview of the equipment's capabilities and its application in the research, evaluation, and development of electronic materials and devices.
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AppNote KEITHLEY: Low Level Measurements Handbook - 7th Edition Precision DC Current, Voltage, and Resistance Measurements

Optoelectronic Study of Nanostructured ZnTe Films for Photovoltaic Applications in CdTe-Type Solar Cells

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Zinc telluride (ZnTe) is a semiconductor with attractive properties for photovoltaic applications, particularly as a hole transport layer (HTL) in CdTe-based solar cells. This material has a bandgap of approximately 2.27 eV and p-type electrical conductivity, characteristics that make it a promising candidate for improving charge transport in second-generation photovoltaic devices.
In this work, the deposition of micro- and nanostructured ZnTe thin films was studied using the Close-Spaced Vapor Transport (CSVT) technique, with the aim of evaluating their potential implementation in solar cells with an FTO/CdS/CdTe/ZnTe/Au:Cu structure. Different deposition conditions were analyzed to promote the formation of nanostructures and to study their behavior in devices both with and without $CdCl_2$ thermal treatment. The resulting films had thicknesses close to 100 nm. Additionally, their optoelectronic and morphological properties were characterized using UV-vis spectroscopy and atomic force microscopy (AFM), respectively. The results demonstrate the potential of ZnTe as an HTL layer in CdTe-based photovoltaic devices.

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Design of a ternary $BiVO_4$/g-C_3N_4/Ti_3C_2 MXene heterostructure for sustainable hydrogen production

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Photoelectrocatalytic hydrogen production is a promising approach for sustainable energy generation [1]. As illustrated in Fig. 1, a ternary $BiVO_4$/ Ti_3C_2-MXene/g-C_3N_4 system is designed to enhance visible-light-driven hydrogen evolution through a Z-scheme heterojunction mechanism. $BiVO_4$ and g-C_3N_4 are employed to construct a heterojunction that promotes efficient charge separation and extends visible-light utilization [2]. Ti_3C_2 MXene is incorporated as a cocatalyst to facilitate electron transport, provide active reaction sites, and suppress charge carrier recombination [3]. The synergistic effect of the heterojunction and the MXene cocatalyst is expected to improve photocatalytic performance. The materials will be characterized using XRD, SEM, FTIR, UV–Vis, and DRS, while their hydrogen production activity will be evaluated under simulated solar irradiation. This work aims to contribute to the development of efficient photocatalytic systems for clean and renewable hydrogen generation.

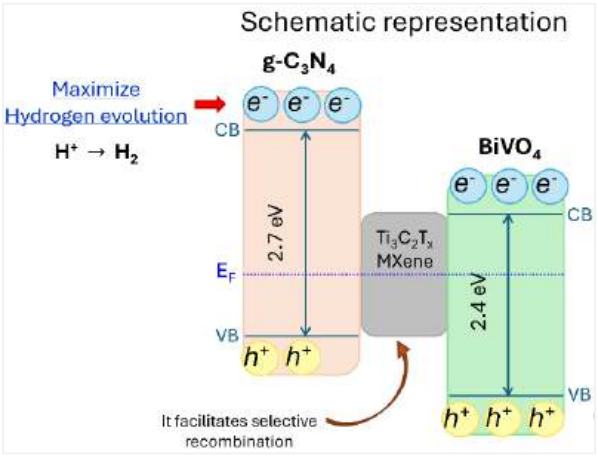

Fig. 1. Schematic illustration of the Z-scheme heterojunction g-C_3N_4/Ti_3C_2-MXene/$BiVO_4$.

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Development of a Ni-free Co-25Cr alloy for the manufacturing of coronary stents

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Cardiovascular diseases remain the leading cause of mortality in Mexico, with acute myocardial infarction (AMI) the most prevalent clinical condition [1]. AMI results from obstruction of the coronary arteries by atherosclerotic plaques, reducing blood flow and compromising myocardial perfusion [2]. The current standard treatment is implantation of coronary stents to restore vessel patency and re-establish adequate coronary circulation [3]. Ongoing advances in interventional cardiology and materials science have led to at least five generations of coronary stents, each designed to enhance mechanical performance, long-term durability, and biocompatibility [4,5]. Recent efforts have focused on nickel-free metallic alloys for cardiovascular devices because nickel may trigger inflammatory and hypersensitivity responses after implantation [6–9]. In this context, the present study highlights the development of a rapidly solidified Ni-free Co–25Cr alloy and describes the technological process route used to fabricate coronary stent prototypes.

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XANTHAN GUM DYNAMICS: PROBING ORDER-DISORDER TRANSITIONS BY HIGH-FIELD NMR RELAXOMETRY

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Xanthan gum's macroscopic performance depends strictly on the supramolecular transition from a rigid double helix to a disordered random coil [1]. Although this shift is driven by temperature and ionic strength, the underlying molecular dynamics remain difficult to characterize [2]. To resolve this, we employed high-field (HF)-NMR relaxometry to probe polymer chain mobility across a broad temperature range. Specifically, measurements of longitudinal (T_1) and transverse (T_2) relaxation times reveal a marked increase in T_2 at the transition temperature (T_m), signaling enhanced conformational flexibility during helical melting. Furthermore, high-field sensitivity allowed for the differentiation of rapid local motions from slower backbone dynamics. Ultimately, these findings establish a direct correlation between microscopic relaxation and the polymer's supramolecular state, thereby providing a robust framework for optimizing xanthan gum in sectors ranging from food stabilization to advanced tissue engineering.

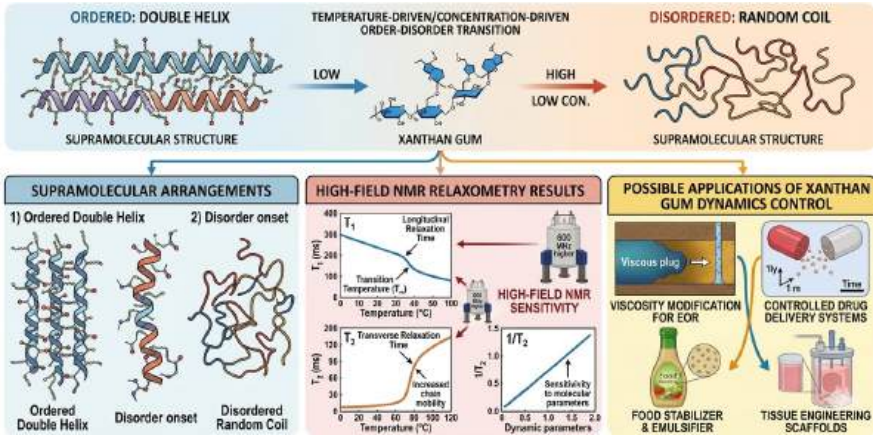

Figure 1. HR-NMR relaxometry tracks the shift from rigid double helices to flexible coils, enabling precision tuning for industrial and medical use.

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FROM THE LABORATORY TO THE ENTERPRISE: NANOTECHNOLOGY WITH AN ENTREPRENEURIAL FOCUS.

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The academic journey, from undergraduate studies to the doctoral level, provides a comprehensive perspective on how scientific research, driven by global collaboration, can be translated into tangible societal benefits. Beyond theoretical frameworks, science possesses an immense potential to generate cutting-edge technology capable of fundamentally transforming our world; it is through applied knowledge that the tools which elevate our quality of life are forged. This disruptive impact is evidenced by the legacy of visionaries who redefined modern industry: Kamerlingh Onnes (helium liquefaction and superconductivity, 1908), Marie Curie (mobile radiography units, 1914), Ernst Ruska and Max Knoll (transmission electron microscope, 1931), Alan Turing (foundations of computer science, 1936), Robert Oppenheimer (atomic energy, 1945), John Bardeen (first point-contact transistor, 1947), Gordon Moore (foundational microprocessors, 1971), Shirley Ann Jackson (telecommunications and optical fiber, 1976), Gerd Binnig and Heinrich Rohrer (scanning tunneling microscope, 1981), Geoffrey Hinton (deep artificial neural networks, 1986), Shuji Nakamura (high-brightness blue LED, 1993), and Jennifer Doudna & Emmanuelle Charpentier (CRISPR-Cas9 gene editing).

The central objective of this talk is to demonstrate that rigorous scientific and academic development is a powerful catalyst for emerging technologies with direct applications in everyday life and the industrial sector. Aligning with this vision of transformative innovation, Dr. León Nataret has made an outstanding contribution to the manufacturing of graphenic materials. By pioneering a green chemistry approach, he has successfully eliminated the use of highly toxic and environmentally harmful reagents, such as $KMnO_4$, $NaNO_3$, and H_2SO_4. Instead, Dr. León Nataret has developed sustainable synthesis methodologies utilizing edible organic waste—specifically nopal and onion peels—as precursors for graphene production. This breakthrough proves that nanotechnology can be simultaneously disruptive, commercially scalable, and ecologically responsible.

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HYDRO-POLYMERIC MATRIX ENRICHED WITH ZINC OXIDE NANOPARTICLES AND PLANT GROWTH-PROMOTING RHIZOBACTERIA TO ENHANCE DROUGHT TOLERANCE IN MAIZE

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Background: Drought is a major constraint to agricultural productivity, causing the accumulation of cytotoxic reactive oxygen species (ROS) and restricting root development. Although plant growth-promoting rhizobacteria (PGPR) can mitigate these effects, efficient, stable, sustainable, and cost-effective seed coating carriers are still needed to ensure microbial viability and enhance plant drought responses [1]. **Aim:** To develop a bioactive hydro-polymeric seed coating formulation for maize and evaluate its ability to promote early rhizobacterial establishment and improve drought tolerance during seedling establishment. **Methods:** A seed coating formulation based on a hydro-polymeric matrix enriched with zinc oxide nanoparticles (ZnO-NPs) and a consortium of four PGPR strains was developed. Coated maize seeds were evaluated under field conditions using a 2 × 4 factorial experiment arranged in a randomized complete block design. Water deficit was imposed at the V3 growth stage, and plants were maintained for 14 days under optimal irrigation or severe drought. Plant growth, root architecture, relative water content, chlorophyll content, oxidative stress, and rhizosphere bacterial colonization were assessed [2]. **Results:** Under severe drought, the hydro-polymeric bioformulation significantly improved maize physiological resilience. Compared with untreated plants, treated plants showed greater vigor, fully expanded leaves, higher turgor, darker green foliage, thicker stems, and more uniform growth, whereas controls exhibited chlorosis, reduced growth, and dehydration symptoms. Compared with untreated controls, treated plants maintained a 32% increase in relative water content (RWC) and a 21% increase in SPAD chlorophyll values, and approximately 60% lower malondialdehyde (MDA) levels, indicating reduced lipid peroxidation and oxidative damage. In addition, the formulation enhanced root development and increased total dry biomass by more than 17%, suggesting improved soil exploration and water uptake during early crop establishment. **Conclusion:** The developed bioformulation represents a simple, stable, and cost-effective seed coating strategy that enhances maize drought tolerance. Further large-scale validation under diverse soil and agroclimatic conditions is needed to support its practical application.

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SYNTHESIS AND CHARACTERIZATION OF A GREEN PHOTOCATALYST DERIVED FROM ORANGE PEEL FOR EVALUATION IN THE DEGRADATION OF AN EMERGING CONTAMINANT.

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Emerging contaminants pose a risk to the environment and human health. Water bodies are deteriorating due to untreated wastewater discharges that facilitate the presence of toxic substances. Consequently, a proposal was developed to create a "green" photocatalyst by repurposing orange peels. The orange peels underwent sequential calcination first at 200°C for one hour and then at 400°C for one hour to transform the biomass into a stable carbonaceous material [1]. Hydrothermal synthesis was then performed to transform the precursors; 3M orthophosphoric acid, 0.502 g of orange-derived carbon waste, and 4.023 g of urea were added to a Parr-type reactor. Stirring was initially set at 350 rpm to promote dispersion, then increased to 1100 rpm at 300°C for three hours. XRD characterization of the resulting material revealed a diffractogram characteristic of hydrochar, consistent with results reported by Antonella Satira et al. in 2021 [2]. Subsequently, photolysis tests were conducted in a photocatalytic reactor using a 10 ppm Diclofenac solution; as no molecular degradation was observed, 0.1517 g of activated carbon was added. The mixture was subjected to adsorption for one hour with stirring at 350 rpm under UV light, with 4 mL samples taken every 30 minutes over a three-hour period. Evaluation of the modified material showed 64% degradation of the Diclofenac within three hours. This proposal is promising as it utilizes waste materials as photocatalysts, modifying their physicochemical properties to eliminate molecules that threaten the environment and the health of living organisms.

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Hydrogen production from a platform molecule via heterogeneous catalysis.

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Rising global energy demand and the need to reduce greenhouse gas emissions have driven the search for clean, sustainable energy sources. In this context, hydrogen has emerged as one of the most promising energy carriers due to its high energy content. Concurrently, glycerol the primary byproduct of the biodiesel industry has attracted growing interest as a platform molecule for producing high-value-added products, including hydrogen. This study evaluates hydrogen (H_2) production from glycerol using layered oxides as heterogeneous catalysts in a reforming reaction, carried out in a Parr reactor fed with varying glycerol/water mixtures. [1]

The material analyzed was sodium zirconium silicate (Na_2ZrSiO_4). Physicochemical characterization of the catalysts was performed using X-ray diffraction (XRD), scanning electron microscopy (SEM), nitrogen adsorption (BET), zeta potential analysis, and isopropanol decomposition reactions. Reforming reactions were conducted in the Parr reactor. Gaseous products were analyzed via gas chromatography, while liquid products were analyzed using infrared spectroscopy (FT-IR).

Sodium zinc silicate (Na_2ZnSiO_4) favored glycerol conversion and produced the highest (H_2) signal intensity in the chromatogram, confirming its high catalytic performance. Finally, the use of layered basic oxides as catalysts represents a promising avenue for glycerol valorization and sustainable hydrogen production, contributing to the reduction of industrial waste and the development of a circular economy focused on the energy transition toward clean, renewable sources. [2]

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Optimization of a Flame-Retardant Polymer Nanocomposite and Its Business Model

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Transitioning from the laboratory to industrial production requires a real market, resource optimization, energy and space savings, and the pursuit of practical and permanent solutions. This study optimized a flame-retardant nanocomposite composed of polyester resin, calcium carbonate, glass fiber, and montmorillonite, the latter chemically modified with a high-molecular-weight amine to render it organophilic montmorillonite, thereby ensuring fine dispersion within the polyester resin matrix (Patent MX 345454). Flame resistance testing was conducted in accordance with ASTM D 5048, while the heat deflection temperature (HDT) was measured following ASTM D-648. The best flame-resistance results were achieved by adding from 20 to 50% calcium carbonate and 10% modified clay; under these conditions, flame resistance ranged from 5 to 12 minutes, with a post-flame time of 0 seconds. At these same proportions, the flame-retardant material raised the heat deflection temperature from 71°C to over 215°C, an increase of slightly more than threefold compared to conventional flame retardants. X-ray diffraction analysis revealed no crystalline regions in the clay, indicating a high degree of dispersion. Since the clay used in the development of the flame retardant was imported, potential substitutes were sought from Mexican mines, involving site visits to the states of Durango, Veracruz, and Hidalgo. Powder X-ray analysis determined that clay from the company Arcillas Industriales de Durango offered the best characteristics to replace the imported material. The amine was purchased from the Chinese company AmityChem at a cost of $3.80, compared to the alternative with a price of $154/kg. A business plan was developed, linking the project to a commercial feasibility study that covered the business model, market sector identification, marketing strategy, and technical, financial, and organizational analyses. The enterprise Nanogenesys Solutions was founded in 2024, and offers a line of three flame-retardant products, listed here with their prices: modified clay (Nefiamit 92) at $298.00 MXN/kg, a flame-retardant nanocomposite (Nefiamit 93) at $255.00 MXN/kg, and flat sheets (Nefilam) at $329.00 MXN/m². The financial study projects an IRR of 19.7% and an initial investment of $2,600,000.00 MXN, with a four-year payback period. The organizational study identified three key operational areas: production, sales, and administration. The nanocomposite's flame resistance exceeds the standard by at least fivefold, while its deflection-under-load resistance is three times higher. The business plan confirmed market demand for the flame-retardant material and identified passenger bus manufacturers as the target business niche. It also established the required investment and payback period, while demonstrating that the material's commercial value is affordable and offers potential advantages for the automotive industry.

Synthesis and characterization of the high-entropy ceramic (Co, Mn, Fe, Cr, Ni, Al) oxide applied to a pressure meter sensor.

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Abstract: Accurate pressure measurement is critical in the aerospace, energy and petrochemical industries. Alumina ceramic sensors are the current standard, but they present limitations under extreme process conditions. This work presents the development of a high-entropy ceramic (HEC) based on an equimolar solid solution of (Co, Mn, Fe, Cr, Ni, Al) oxides [1] for application in high-precision pressure meter sensors.

The synthesis was performed using the chemical coprecipitation method from nitrates dissolved in water, aiming to maximize homogeneity and reduce phase formation temperatures compared to traditional solid-state methods. The thermal evolution of the system was monitored by Thermogravimetric Analysis (TGA) and Differential Thermal Analysis (DTA), identifying a critical mass stabilization (70 % loss) and a phase transition near 900°C. X-ray Diffraction (XRD) confirmed the structural transition of the material from an essentially amorphous state at room temperature to the consolidation of a single high-entropy spinel phase between 900°C and 1000°C. This was evidenced by the narrowing of the Bragg reflections and the adjustment of lattice parameters. Additionally, Scanning Electron Microscopy (SEM) allowed the observation of morphological evolution from irregular and porous agglomerates in the precursor to define microstructures after thermal treatment. Finally, the material is sintered and evaluated through Vickers micro-hardness tests, flexural strength (3-point), and fracture toughness estimation to guarantee its mechanical integrity and long-term metrological stability in hostile environments.

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Abstract preparation

Development of a solar nano-photocatalytic process for hydrogen production and separation, using emerging contaminants as sacrificial agents.

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Emerging contaminants from pharmaceutical drugs continuously enter aquatic environments, largely because conventional waste treatment falls short in removing them [1]. Given this persistent problem, we need viable technologies that can break down these pollutants. Solar photocatalysis offers a compelling post-treatment alternative, especially for small wastewater treatment plants, where it can drive the conversion and eventual mineralization of stubborn organic compounds. One of the emerging contaminants that we focus on is drugs, since the pharmaceutical industry is the one that generates this type of contamination the most together with the population [2], among them is ibuprofen, which is very commonly used drug worldwide, is an anti-inflammatory that can ease pain, fever, and more symptoms [3]Li et al., 2021). In the research. In this research we design and develop renewable technology, a solar photocatalytic capable of degrading emerging contaminants from pharmaceutical origin. The aim of this study is to have an alternative to reduce the environmental impact and with a low cost for small wastewater treatments plants, employ TiO_2 dopped with Ag to increase the photodegradation reaction. The results showed a 70 % and 75 % decrease of Total Organic Carbon at use of TiO_2 and TiO_2/Ag respectively. Both values, 70 % and 75 %, mean that TiO_2 promotes the ibuprofen degradation. Additionally, the TiO_2/Ag and TiO_2 treatment obtained a similar degradation measure by Chemical and Biochemical Oxygen Demand.

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Abstract preparation

Synthesis of MXene ($Ti_3C_2T_x$)/(ZIF-67) nanocomposites for electrocatalytic applications.

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The development of efficient and cost-effective electrocatalysts is fundamental for the transition to clean energy storage and conversion technologies [1]. This work presents the design and synthesis of nanocomposites based on metal-organic frameworks (ZIF-67) and two-dimensional titanium carbide MXene supports ($Ti_3C_2T_x$), aimed at the electrocatalysis of the oxygen evolution reaction (OER) and oxygen reduction reaction (ORR). In the first step, the MXene support was obtained from the exfoliation of the precursor MAX phase (Ti_3AlC_2) through a selective etching process with hydrofluoric acid, resulting in a multilayer structure with high conductivity and hydrophilic surface terminations. Separately, the crystalline ZIF-67 phase was synthesized using a microwave-assisted method, a strategy that reduced reaction times and promoted a homogeneous nucleation of the cobalt particles. For the formation of the nanocomposite, both materials were dispersed in methanol and integrated through magnetic stirring, followed by homogenization with an ultrasonic probe to ensure a uniform distribution and optimize the interfacial interaction.

The structural synergy between the metallic conductivity of the $Ti_3C_2T_x$ and the porosity of ZIF-67 promotoes a greater exposure of active sites ($Co-N_4$) and facilitates charge transfer [2]. The electrocatalytic activity of the OER and ORR was evaluated by voltammetry techniques in a three-electrode cell, through which the overpotentials, Tafel slopes, and electrochemical stability of the composite material were obtained.

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THE MULTIPLE PROPERTIES OF MULLITA-Ag CERMETS AND ITS POTENTIAL APPLICATIONS

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Mullite-Ag cermets, an emerging class of hybrid materials combining the thermal and chemical stability of mullite ceramics with the conductivity and functional properties of silver, were developed. In this work, Mullite-Ag cermets were sintered by high-energy milling and controlled sintering, varying the silver content from 1 to 30% at two sintering temperatures, 1500 and 1600 °C. Initial studies show that the incorporation of silver increases density and reduces porosity, with grain size increasing as the silver concentration increases and a more homogeneous microstructure. Mechanically, Mullite-Ag cermets maintain thermal shock resistance and low thermal expansion, while silver provides greater toughness and ductility, mitigating the typical brittleness of ceramics. Electrically, resistivity decreases significantly, and the activation energy for conduction is reduced, making them suitable for use in sensors and devices subjected to high temperatures. The combination of chemical stability and electrical conductivity positions Mullite-Ag cermets as candidates for electronic components, refractories in the aerospace and automotive industries, and corrosion-resistant materials in chemical and environmental processes.

University-industry collaboration is not just about signing agreements, but about being able to propose versatile materials that can meet the diverse requirements of the industrial sector. In this sense, the set of Mullite-Ag cermets developed constitutes a versatile and high-performance alternative, capable of responding to the demands of strategic sectors. Their development confirms the potential of ceramic-metal hybrid materials as innovative solutions for contemporary science and technology.

Performance of l-proline and leucine compounds as corrosion inhibitors for Ni-Nb metallic glass in a 3% NaCl solution.

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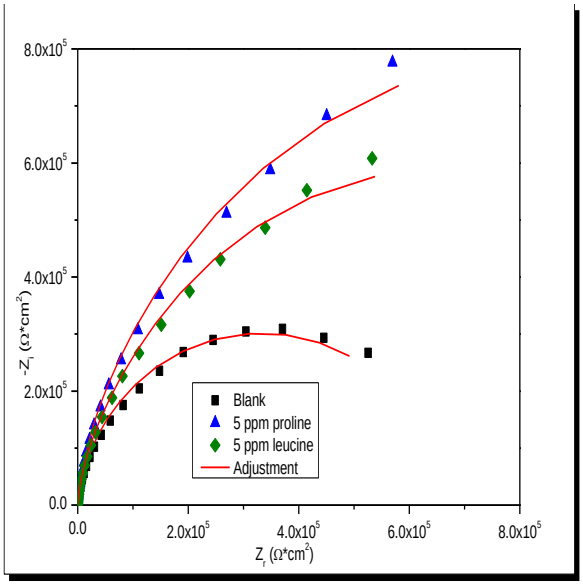

Metallic glasses are materials characterized with an amorphous atomic structure similar to that of ordinary glass, but composed of a metal alloy. They are typically produced through rapid solidification techniques [1]. In this study, examines the compounds L-proline and leucine as potential corrosion inhibitors for a Ni-Nb metallic glass strip; although it has been demonstrated that these types of materials exhibit high corrosion resistance in chloride solutions, they can still show signs of localized corrosion on their surface [2]. The electrochemical analysis was performed using Electrochemical Impedance Spectroscopy (frequency range from 10 mHz to 10 kHz, sinusoidal perturbation amplitude of 10 mV, and 10 points per decade) and Potentiodynamic polarization measurements (potential range: ±300mV) using a three electrode electrochemical cell consisting (reference: saturated calomel electrode, counter electrode: graphite, and working electrode: metal-coated glass strips with an area of 0.3 cm^2). The EIS data were analyzed using equivalent electrical circuits. The results showed efficiency percentages greater than 90% for each one of the inhibitors, indicating that L-proline and L-leucine effectively reduced the corrosion rate of the Ni–Nb metallic glass in the 3% NaCl solution.

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Hydrogen Production from the Photocatalytic Degradation of Emerging Contaminants

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Water contamination by organic compounds and the need to develop cleaner energy sources have driven the search for materials capable of efficiently utilizing available radiation. Photocatalysis makes it possible to use light energy for both pollutant degradation and hydrogen production. However, conventional photocatalysts such as TiO_2 and ZnO mainly absorb in the ultraviolet region because of their wide band gaps, which limits the use of visible radiation **[1]**.

In this context, copper bismuthate ($CuBi_2O_4$) represents an attractive alternative due to its ability to absorb visible light, associated with a band gap of approximately 1.5–1.8 eV. In addition, bismuth-based materials exhibit relatively low toxicity. These characteristics have led $CuBi_2O_4$ to be investigated for applications related to pollutant treatment, hydrogen production, and solar energy utilization **[2]**.

Despite these advantages, the performance of $CuBi_2O_4$ can be limited by the behavior of the charge carriers generated during irradiation **[2]**. Therefore, this work proposes its combination with CuO to form a $CuBi_2O_4$/CuO material, aiming to complement the properties of both oxides and enhance their photocatalytic response under visible-light irradiation **[3]**.

The developed material is studied in relation to two current challenges: water pollution and the search for cleaner energy-generation alternatives. Its performance is evaluated through the degradation of Rhodamine B and photocatalytic hydrogen production. With this approach, the work aims to demonstrate the potential of semiconductor material design for environmental and energy applications related to water treatment and solar energy utilization **[2,3]**.

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Abstract preparation

Development of ZnO Nanoparticle-Reinforced Aloe Vera Biopolymer Matrix for Concentrated Berrycactus Juice Delivery: Physicochemical Characterization and Preliminary Vascular Evaluation.

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Arterial hypertension is a leading cause of premature mortality worldwide. Previous *ex vivo* studies demonstrated that concentrated berrycactus juice (CBJ) induces significant vasorelaxation in aortic rings from hypertensive rats, achieving nearly 100% relaxation at 75 mg/mL. Building on these findings, a biopolymeric matrix enriched with zinc oxide (ZnO) nanoparticles (NPs) is being developed as a potential platform for the controlled delivery of CBJ. However, the effects of the individual components of this system on vascular tone regulation remain unclear. This study aimed to synthesize and characterize an Aloe vera-based biopolymeric matrix and ZnO NPs, and to evaluate their vascular effects. Fourier-transform infrared spectroscopy (FTIR) analysis revealed the presence of various functional groups within the compounds; for the biopolymer matrix, COO^{-}, COH, C-O, C-H and O-H groups were identified, corresponding to its organic phase. In the case of ZnO NPs, the functional groups present were COO^{-}, C-O, O-H and Zn-O, which are characteristic of ZnO. Finally, the CBJ exhibited C-H, C=C, O-H, C-O, C-N and C=O functional groups, consistent with its complex composition of bioactive organic compounds. X-ray diffraction (XRD) analysis indicated a predominantly amorphous profile for the biopolymeric matrix, consistent with its organic composition, while ZnO NPs exhibited the characteristic wurtzite crystalline phase. Scanning electron microscopy (SEM) revealed a spherical morphology for the ZnO NPs, with an average particle size of 15.8 ± 4 nm and a relatively homogeneous porous morphology of the biopolymeric matrix. Vascular activity was evaluated in 3-mm thoracic aortic rings isolated from male Wistar rats (200-220g) and pre-contracted with phenylephrine. The biopolymeric matrix at 0.3, 1, 3, and 30 mg/mL and ZnO NPs at 0.3, 3, 30, and 60 µg/mL did not significantly alter vascular tone. In contrast, CBJ at 5.5 and 11 mg/mL induced more than 75% vasorelaxation. These results demonstrate the vascular compatibility of the biopolymeric matrix and ZnO NPs at the tested concentrations and confirm the pronounced vasorelaxant activity of free CBJ. Collectively, these findings support further development and evaluation of the CBJ-loaded ZnO/biopolymer composite as a potential controlled-delivery system.

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Solar Panel Waste Valorization under a Circular Economy Approach

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The deployment of renewable energy technologies has increased significantly due to the need to reduce greenhouse gas emissions produced by the combustion of fossil fuel. In this context, it is estimated that nearly 80% of primary energy is used to meet global energy demand, highlighting the importance of these technologies in the energy transition [1]. In Mexico, photovoltaic systems began to be implemented in the 1980s; therefore, waste from the first installed systems is currently being generated, considering a service life of 25–30 years [2]. It is projected that by 2045, approximately 690,907 m³ of photovoltaic waste will be generated [3]. However, current regulations regarding its management remain ambiguous, making the adoption of circular economy strategies essential.

The present work aims to evaluate valorization routes for solar panel waste and their derivatives from treatments processes, under a circular economy approach, to reduction waste generation from renewable technologies. Previous studies by Negrete et al. [4,5] optimized a thermal treatment for component separation, achieving reductions in processing time and energy consumption compared to conventional methodologies.

Based on physicochemical characterization and the estimation of materials generated during thermal treatment for a conventional 1 MWp photovoltaic plant (with 505 W modules), as shown in Figure 1, two main scenarios were identified: functional solar panels and damaged panels.

Based on these scenarios, the circular economy taxonomy (9R framework) was applied [6], defining three key strategies: Remanufacturing, Repurposing, and Recycling. Results indicate that strategies focused on remanufacturing and repurposing offer greater sustainability and economic viability compared to conventional recycling.

This approach provides a foundation for the development of sustainable photovoltaic waste management strategies with strong potential for industrial implementation.

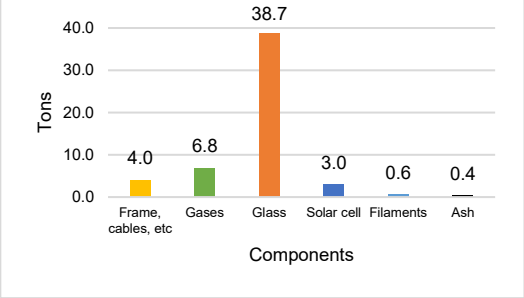

Figure 1. Tons of waste generated from a solar farm

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Lead oxide nanoparticles: evaluation of the toxicity of the tetragonal allotropic structure versus the orthorhombic structure

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Lead oxide nanoparticles have a wide range of applications. For example, they have been used as catalysts in water purification by degrading methyl orange, a common dye in wastewater. Lead oxide is also used in the production of lead-glazed ceramics. During the ceramic manufacturing process, an important step is the annealing of the clay, in which high temperatures of approximately 400–600 °C are reached [1]. At these temperatures, a transition occurs in the crystal structure from tetragonal (α-PbO) to orthorhombic (β-PbO). In this work, tetragonal and orthorhombic nanoparticles were synthesized by chemical precipitation. Furthermore, their toxicity was investigated using oxidative stress biomarkers in rainbow trout organs. The results revealed the non-toxicity of both allotropic forms of lead oxide nanoparticles (as shown in Figure 1). The effect may be due to acute exposure and the micrometric size of the nanoparticles [2].

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Ecological synthesis of silver nanoparticles using aqueous extracts of *Ricinus communis*.

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Plant secondary metabolites play protective and defensive roles against invading organisms. While not essential for plant survival, they have diverse applications, including their use as anticancer agents, pesticides, and in food production. Among these metabolites are polyphenols, characterized by their anti-inflammatory and antioxidant properties, which help protect cells against oxidative stress. Recent reports show the potential use of polyphenols for the biosynthesis of nanoparticles with different composition, shape, and crystalline structure. The aim of this work is to prepare aqueous extracts with a high polyphenol content from *R. communis* seeds and also to evaluate their potential as reducing and stabilizing agents for the synthesis of silver nanoparticles. The aqueous extract of *R. communis* (red spectrum) was characterized by FTIR, where the black spectrum corresponds to gallic acid (a standard polyphenol) and has many peaks, including the characteristic peak at 1699 cm^{-1} due to the carbonyl vibration ν(C=O) and carboxylic acids [1], as shown in Figure 1a. The *R. communis* extract successfully synthesized silver nanoparticles, whose hydrodynamic diameter was 2000 nm, as can be seen in the spectra in Figure 1b, obtained by dynamic light scattering.

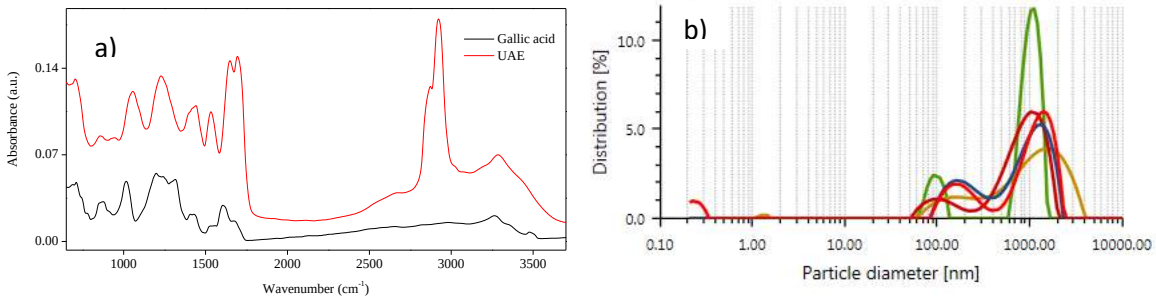

Fig 1. FTIR spectral behavior of gallic acid (black line) and of *R. communis* extract (red line) and b) silver nanoparticle size in solution.

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Biomimetic Membranes Derived from Fish Scales for Bone Regeneration: In Vitro and In Vivo Evaluation and the Impact of Sterilization on Structure–Property Relationships

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Fish scales are a natural source of collagen and hydroxyapatite with significant potential for the development of biomaterials for bone regeneration. In this study, fish scale-derived membranes were developed by taking advantage of their natural composition and structural organization to obtain biomimetic materials with promising physicochemical and biological properties.

The membranes were characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and scanning electron microscopy (SEM) to evaluate their chemical composition, thermal stability, structural organization, and surface morphology. These analyses were performed before and after sterilization to determine the effect of the sterilization process on the structure and properties of the biomaterial.

The results confirmed the presence of characteristic collagen functional groups and hydroxyapatite-associated signals. Furthermore, sterilization induced changes in intermolecular interactions and structural organization while preserving the overall integrity of the membranes. Biological evaluation using mesenchymal stem cells demonstrated favorable cell viability and biocompatibility. In addition, in vivo studies revealed a positive biological response and tissue integration, supporting the potential of these membranes for regenerative applications.

Overall, the findings highlight fish scales as a sustainable and promising raw material for the development of biomimetic membranes for bone regeneration and provide valuable insights into the influence of sterilization on structure–property relationships.

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Acknowledgements (10 pt)

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X-ray Spectroscopic Investigation of the Electronic Structure of Au Nanoparticle-Modified TiO_2 Films for Dye-Sensitized Solar Cells.

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Dye-sensitized solar cells (DSSCs) represent a low-cost alternative for solar energy conversion [1]. The electronic structure of anatase TiO_2 films containing 0, 1.5, 3, and 6% Au nanoparticles was investigated both in the presence and absence of dye. The samples were studied by XAS, XES, and RIXS at beamline 8.0.1 of the Advanced Light Source [2], focusing on the Ti $L_{2,3}$ and O K-edges. TEY and TFY detection modes enabled surface-sensitive changes to be distinguished from those occurring in the bulk. XAS revealed that Au nanoparticles induce a nonlinear modification of Ti 3d states with t_{2g} and e_g symmetry and their hybridization with O 2p states. In the absence of dye, Au concentrations of 1.5 and 3% produced the most pronounced surface modifications, whereas at 6% Au the density of unoccupied states increased again. Differences between TEY and TFY indicate that these effects occur predominantly at the surface, while XES revealed modifications in the occupied electronic states. RIXS enabled the identification of d–d excitations associated with Ti^{3+} sites as well as charge-transfer processes. In the absence of dye, the intensity of these excitations increased with increasing Au content; upon sensitization, the spectral weight was redistributed toward lower-energy excitations and charge-transfer channels, suggesting partial delocalization of the d–d excitations. These results provide insights into the electronic-structure effects of Au nanoparticles and contribute to the rational design of plasmonic photoanodes for DSSCs.

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Estructura electrónica de películas de TiO_2 con nanopartículas de Au para celdas solares sensibilizadas con tinte investigadas mediante espectroscopías de rayos X.

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Las celdas solares sensibilizadas por tinte (DSSC) constituyen una alternativa de bajo costo para la conversión de energía solar [1]. Se investigó la estructura electrónica de películas de TiO_2 anatasa con 0, 1.5, 3 y 6 % de nanopartículas de Au, en presencia y ausencia de tinte. Las muestras se estudiaron mediante XAS, XES y RIXS en la línea 8.0.1 del Advanced Light Source [2], analizando las orillas $L_{2,3}$ del Ti y K del O. Los modos TEY y TFY permitieron diferenciar los cambios superficiales de los producidos en el volumen. XAS mostró que el Au modifica de manera no lineal los estados Ti 3d de simetría t_{2g} y e_g y su hibridación con O 2p. Sin tinte, 1.5 y 3 % de Au produjeron los cambios superficiales más pronunciados, mientras que con 6 % aumentó nuevamente la cantidad de estados desocupados. Las diferencias entre TEY y TFY indican que el efecto ocurre predominantemente en la superficie; XES reveló modificaciones en los estados ocupados. RIXS permitió identificar excitaciones d–d asociadas con sitios Ti^{3+} y procesos de transferencia de carga. Sin tinte, su intensidad aumentó con el contenido de Au; el sensibilizador redistribuyó el peso espectral hacia menores energías y canales de transferencia de carga, lo que sugiere una deslocalización parcial de las excitaciones d–d. Estos resultados contribuyen al diseño de fotoánodos plasmónicos para DSSC.

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DEVELOPMENT AND OPTIMIZATION OF A LIPID NANOPARTICLE-BASED TOPICAL DELIVERY SYSTEM CONTAINING TEA TREE OIL AND CURCUMIN FOR ACNE TREATMENT

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Abstract

Acne vulgaris is a chronic inflammatory disease of the pilosebaceous unit characterized by excessive sebum production, proliferation of *Cutibacterium acnes*, and persistent skin inflammation. Although conventional topical therapies are effective, they frequently cause adverse effects such as skin irritation, bacterial resistance, and poor patient adherence. Lipid nanoparticle-based drug delivery systems have emerged as promising alternatives because they enhance the stability, protection, and controlled topical delivery of bioactive compounds [1,2,4].

The aim of this work is to develop and optimize lipid nanoparticle-based formulations containing tea tree oil and curcumin for topical acne treatment. Nanoparticles were produced by high-shear homogenization using glyceryl behenate as the solid lipid, PEG-32 lauroyl glycerides as an emulsifying lipid excipient, and different stabilizing agents. Preliminary studies evaluated the influence of homogenization cycles, lipid composition, and stabilizer type on particle size, physical stability, and curcumin encapsulation efficiency. Curcumin content was determined by UV-Vis spectrophotometry at 420 nm.

Preliminary results demonstrated that processing conditions and formulation composition markedly influenced the physicochemical characteristics of the nanoparticles. Increasing the number of homogenization cycles promoted particle size reduction, whereas lipid composition affected curcumin encapsulation efficiency. Furthermore, Poloxamer 188 exhibited superior physical stability compared with other stabilizers evaluated. The analytical method showed suitable linearity and reproducibility for curcumin quantification.

Current work focuses on the optimization of formulation and process variables using a Box-Behnken experimental design to identify the combination of factors that provides optimal physicochemical characteristics. The optimized lipid nanoparticle formulation is expected to improve the topical delivery of tea tree oil and curcumin, representing a promising strategy for the treatment of acne vulgaris.

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Sustainable Polylactic Acid/Cellulose Biocomposites for Packaging: Process Optimization and Energy Consumption

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Developing sustainable polymeric materials requires not only replacing fossil-based plastics with renewable alternatives, but also optimizing their processing and end-of-life performance [1-3]. In this work, cellulose extracted from sawdust, an abundant lignocellulosic by-product, was incorporated into poly(lactic acid) through reactive extrusion using maleic-anhydride-grafted PLA (PLA-g-MA) as a compatibilizing agent. An extreme-vertex mixture design was employed to evaluate the effect of cellulose and PLA-g-MA content on the structural, mechanical, thermal, rheological, biodegradation, and processing energy features of the resulting biocomposites. The optimal formulation, containing PLA/PLA-g-MA/cellulose, maintained the tensile strength of the neat PLA while improving hardness and Young´s modulus.
In addition, the composite exhibited enhanced biodegradability compared with the pure PLA. Energy consumption during extrusion was 1.68 kWh/kg, a moderate increase relative to neat PLA (1.11 kWh/kg) but still 5.6% lower than that of low-density polyethylene. The results demonstrate that reactive extrusion provides an effective route for valorizing sawdust-derived cellulose into high-performance biodegradable PLA biocomposites without compromising processability or mechanical performance. This approach highlights the potential of biomass-derived fillers for developing more sustainable materials for packaging and food-service applications.

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VALORIZATION OF PINE SAWDUST AS A CELLULOSE SOURCE FOR SUSTAINABLE POLYMERIC MATERIALS

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Abstract

The valorization of lignocellulosic residues as renewable sources for cellulose-based materials has gained increasing attention as a sustainable alternative to conventional polymeric materials. In this work, pine sawdust was investigated as a low-cost cellulose source through sequential alkaline (sodium hydroxide, NaOH) and alkaline-peroxide (sodium hydroxide/hydrogen peroxide, $NaOH/H_2O_2$) treatments. Sawdust was first treated with 0.1 M NaOH to remove non-cellulosic components [1], followed by treatment with $NaOH/H_2O_2$ treatment using different reagent volumes and temperatures to promote enhanced delignification and removal of extractives [2-3]. An experimental design based on response surface methodology, comprising 13 trials, was developed and subsequently executed to evaluate the effect of treatment conditions on cellulose yield. Cellulose yields ranged from 46.0 to 79.16%, with the highest yield obtained using 80 mL of $NaOH/H_2O_2$ at 50 °C after 4 h of treatment. The center points of the experimental design – using 50 mL of $NaOH/H_2O_2$ at 65 °C – showed yields between 53.0 and 58.0%. The resulting cellulose-rich fractions were evaluated using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC). FTIR confirmed the persistence of cellulose I, with lignin and hemicellulose-related signals. XRD confirmed the persistence of cellulose I, with crystallinity ranging from 30.53 to 74.17%.TGA/DSC revealed modified degradation profiles and enhanced thermal stability in selected treatments. Overall, the results demonstrate that treatment conditions strongly influence cellulose recovery, structural organization, and thermal stability, highlighting pine sawdust as a promising feedstock for obtaining cellulose-rich materials and sustainable polymeric composites.

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Effect of keratin fiber oxidation on flame-retardant polymer biocomposites

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The use of flame-retardant additives in polymer biocomposites has diversified their applications, enabling the replacement of conventional synthetic polymer materials. The mineral base additives are the most worldwide used flame-retardants, due to low cost and broad availability; however, they must be used in high concentration, most commonly at 55-65 % and sometimes even up to 80 % depending on the polymer matrix, which can negatively affect mechanical properties [1]. One alternative to this problem is the use of keratin fibers (KF) derived from tannery industry wastes; these act as mechanical reinforcements. Additionally, the use of KF contributes to reducing the flame-retardant additive content, improving mechanical properties and contributing to the production of sustainable biocomposites through the optimization of compounding variables [2].

The modification of natural fibers has been used as an alternative to increase interfacial adhesion and improve the mechanical interlocking between the polymer matrix and the fiber [3]. Regarding KF, the oxidation process can modify the functional groups present on their surface, promoting the formation of chemical and physical interaction with the polymer matrix [4]. The present work focuses on the development of a polymer biocomposite based on thermoplastic starch, ammonium polyphosphate and modified KF using sulfuric acid and hydrogen peroxide. The KF modification process was optimized by considering exposure time, concentration and KF length as independent variables to minimize the total flaming time and maximize mechanical properties. The KF were characterized using scanning electron microscopy and FTIR spectroscopy, while the biocomposites were characterized using tensile test, UL94-V test and rheology. The oxidation process in KF revealed the formation of amide I groups due to cleavage of polypeptide chains, as well as the possible breakage of disulfide bonds, which resulted in a reduction in total flaming time.

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MODIFICATION OF A DETERMINISTIC MODEL TO PREDICT THE FINAL HARDNESS OF 6061 ALUMINUM ALLOY TO INCLUDE COOLING RATE DURING QUENCHING PRIOR TO AGING

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The use of aluminum alloys has increased significantly, leading to a growing interest in their study. A key industrial process is precipitation hardening, which enhances the mechanical strength of heat-treated aluminum alloys; this process, also referred to as aging, consists of three stages: solubilization, quenching and aging [1].

In this work, the deterministic model proposed by Myhr and Grong [2], which predicts hardness after aging, was modified to account for the effect of the cooling rate during quenching. To validate the modified model, Jominy end-quench tests were performed on reduced-scale (3:4 ratio relative to the standard) 6061 alloy probes. Each probe, instrumented with three type "K" thermocouples, was solutionized at 530 °C for 2 hours prior to quenching. Subsequently, the Brinell hardness profile was measured along the axial axis on two parallel surfaces of the probe. Finally, the probe was aged at 200 °C for four different time intervals (30, 60, 120, and 240 minutes) and the Brinell hardness profile after aging was measured. Since only three cooling curves were recorded experimentally, a computational code was developed to compute the cooling response throughout the entire probe, thereby obtaining the cooling rate during quenching at each hardness indentation position.

The Myhr and Grong model [2] was modified to incorporate the cooling rate during quenching by modifying its pre-exponential factor. The computed results provided a good approximation of the cooling rate effect during quenching on the final hardness after aging, validating the modified model. Future work will focus on applying this approach to other aging temperatures.

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Physicochemical and microstructural characterization of a porous archaeometallurgical slag from Nuevo Urecho, Michoacán

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The study of archaeometallurgical slags using materials characterization techniques provides information about the thermal and solidification processes associated with ancient metallurgical production. In this work, a foam-like slag sample from Nuevo Urecho, Michoacán, was comprehensively characterized to establish relationships among its composition, crystalline structure, microstructure, physical properties, and thermal behavior.

The sample was analyzed by X-ray fluorescence to determine its bulk elemental composition; X-ray diffraction to identify its crystalline constitution; scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy to examine its morphology and compositional distribution at the microscopic scale; differential scanning calorimetry to evaluate its thermal response; and density measurements as a complementary physical property.

The combined results characterized the sample as a heterogeneous, multiphase material with a porous structure and microstructural features associated with high-temperature transformation, flow, and solidification processes. The chemical, crystallographic, microstructural, and thermal information showed consistent correspondence and supported an integrated interpretation of the formation of the material.

These results demonstrate the value of combining complementary analytical techniques in the study of complex archaeometallurgical materials and contribute to the understanding of the metallurgical technology developed in western Mexico.

Keywords: archaeometallurgical slag, Nuevo Urecho, materials characterization, microstructure.

FIVE LUMPED KINETIC MODELLING OF THE HYDRO-COPROCESSING OF *Jatropha Curcas L.* OIL AND GASOIL BLEND TO GET GREENER AND CLEANER LIQUID HYDROCARBONS

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Heavy oil upgrading has been the challenge for refiners in the last two decades due to the difficulty of treating bulky molecules and emitting pollutands to the enviroment(1, 2). One alternative is mixing vegetable or animal oil to make the processes cleaner and greener . Hence, the present research investigated the kinetis for the hydro-coprocessing of a mixture of 20 vol.% of *Jatropha Curcas* L. oil and 80 vol. % of a 50 vol.% of LGO (Light Gasoil) and HGO (Heavy Gasoil) gasoil blend to get hybrid diesel-like fraction. Catalytic studies were conducted at batch conditions (360, 380, and 400 °C, 6 MPa of initial hydrogen pressure, and 1, 2, 3, and 4 h of reaction time). A sulided Ni-W catalyst supported on Al-SBA-15 with Al/Si molar ratio of 0.05 and the overall metallic content was 30.5 wt.% (5.5 wt.% of NiO, 25 wt.% of WO_3) was used. A five lumped kinetic model was proposed for the following fractions: Residue, Gasoil, Diesel, Kerosene, and Naphtha. According to the power law model, Residue and Gasoil reaction orders were about 2 and 1.4, respectively. Therefore, the Residue and Gasoil were the more complex fractions in terms of their components, so the power a higher than one reaction order represented that simultaneous reactions occurred during the hydrocroprocessing of the heavier componentes of the reaction mixture (triglycerides, free fatty acids, oxygenated, and heavy hydrocarbons in HGO). Activation energies were within the range of 55 to 80 kJ mol^{-1} and the kinetic rates the diesel-like fraction were higher than those for lighter fractions. Kinetic parameters are within the range of previously reported and similar works (3-5). Accordingly, the sulifed Ni-W catalysts supported in Al-SBA-15 mesostructured materiales promoted the diesel-like fraction due to the moderate HCK and HDO of the heavier componentes of the reaction mixture.

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VALORIZATION OF CHEESE WHEY VIA A LOW-COST THERMAL PROCESS FOR LACTOSE RECOVERY

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Artisanal cheese production generates whey with a high organic load, and in many rural areas, small-scale producers lack access to membrane technologies or advanced wastewater treatment systems [1,2]. In this work, we explored a low-pressure physicochemical process to treat semi-acid cheese whey obtained after protein coagulation in Jamay, Jalisco, aiming to recover both reusable reagents and a carbohydrate-rich crystalline fraction. The raw whey, with an initial pH of 5.40 and a biochemical oxygen demand of 40,260 mg/L, was neutralized with carbonate, heated to 95 °C, filtered at atmospheric pressure, and subsequently treated with activated carbon and an alcohol-based precipitation step. The resulting fractions were characterized using Fourier-transform infrared spectroscopy, X-ray diffraction, UV-visible spectroscopy, and scanning electron microscopy. The treatment yielded a colorless aqueous fraction with pH 6.9 and a biochemical oxygen demand of 153 mg/L, corresponding to an apparent reduction of 99.62%. In addition, a crystalline fraction was recovered at approximately 8 g/L. FTIR and XRD analyses suggested the presence of hydrated lactose, together with galactose and calcium DL-lactate pentahydrate. Carbonate, alcohol, and activated carbon recoveries were 90%, 70%, and 95%, respectively. Overall, these findings suggest that a relatively simple process can be useful for reducing the organic load of cheese whey while recovering reagents and lactose-containing solids. However, before considering scale-up or potential agricultural reuse of the treated water, further analytical validation, improved purification of the crystalline fraction, and a complete regulatory assessment of the effluent are still required.

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VALORIZATION OF CHEESE WHEY VIA A LOW-COST THERMAL PROCESS FOR LACTOSE RECOVERY

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Towards energy-efficient processing of lead-free electroceramics through high-energy mechanical activation

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Abstract

High-energy mechanical milling offers an effective approach to improve powder characteristics by reducing particle size, promoting deagglomeration and homogenization, and increasing the contact area between precursor particles. These effects enhance solid-state reactivity and facilitate subsequent synthesis and densification. In this work, high-energy mechanical milling was investigated to optimize the processing of lead-free ceramics through enhanced precursor reactivity.

The effects of milling time and grinding-media size were evaluated through thermal, structural, and microstructural characterization. Mechanical activation promoted particle deagglomeration, improved contact between the precursors, and shifted CO decomposition toward lower temperatures. Milling for 6 h using 3 mm ZrO_2 balls provided the most effective activation conditions. Consequently, formation of the BCTZ perovskite phase was detected at temperatures as low as 700 °C, while phase-pure powders were obtained at 900 °C. Moreover, the processing route also influenced the functional response, with conventionally processed ceramics reaching a piezoelectric coefficient (d_{33}) of 232 pC/N. These results demonstrate that high-energy mechanical activation enhances solid-state reactivity and reduces the thermal requirements preserving competitive functional properties, highlighting its potential as an energy-efficient processing route.

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Vanadium Oxide Thin Films as Advanced Catalysts with Potential Application in Photo-Electrochemical Energy Technologies

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This study addresses the critical challenge of climate change mitigation by advancing the science of clean energy generation and storage, focusing on green hydrogen as a main sustainable energy carrier[1]. The primary objective of this work was to evaluate the viability of nano-crystalline vanadium oxide (VOX) thin films as high-efficiency catalysts to optimize water electrolysis and photo-electrochemical splitting processes. Thin films were synthesized via the low-cost ultrasonic spray pyrolysis technique, using vanadyl acetylacetonate as the chemical precursor[2].

Structural and optical characterization utilizing X-ray diffraction (XRD) and UV-Vis spectroscopy confirmed the successful formation of distinct crystalline VO2 and V2O5 semiconductor phases with band gaps tuned between 2.2 and 2.6 eV. Subsequent electrochemical evaluations via cyclic voltammetry and chronoamperometry demonstrated excellent stability, pronounced photoactivity, and favorable catalytic behavior tailored for hydrogen evolution reactions.

Notably, films processed at deposition temperatures of 350°C and 400°C yielded the highest hydrogen production rates at lower electrical operating potentials, significantly reducing energy penalties before transitioning to conventional electrolytic mechanisms at higher potentials [3]. In conclusion, the structural, optical, and electrochemical properties of these temperature-tuned VOX films highlight their potential as effective, accessible materials for green hydrogen devices, directly contributing to the technological advancement of renewable energy systems and transition storage media.

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FROM MAGNESIUM TO CALCIUM: IDENTIFYING THE KEY LIMITATION IN NATIVE-PH LITHIUM EXTRACTION WITH IL–TOPO SYSTEMS

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Lithium recovery from Andean salar brines is constrained not only by magnesium but also by calcium, whose role under competitive multication conditions remains poorly understood.[1] Conventional divalent-cation removal relies on evaporative concentration and brine basification, which are undesirable when water conservation and brine reinjection are priorities.[2] Here, a β-diketonate ionic liquid (IL) combined with TOPO in the industrial diluent Escaid 110 was evaluated for selective divalent-cation removal and lithium extraction at the native pH of synthetic brines, including a five-cation Maricunga-type composition. Under monovalent conditions, lithium extraction exceeded 90% in less than 3 min, with negligible Na^+/K^+ co-extraction, while McCabe–Thiele analysis predicted approximately 97% Li recovery in two stages. In multicomponent brines, magnesium preferentially occupies the organic phase, whereas increasing TOPO loading promotes calcium uptake and progressively suppresses lithium extraction. Slope analysis indicates that the observed selectivity results primarily from competitive loading rather than intrinsic extraction preference. Carbonate stripping enabled the recovery of up to 71% of Li from the Li-loaded organic phase and up to 97% Ca and 75% Mg from the divalent-loaded phase in a single contact. ^{1}H-NMR confirmed the structural integrity of the extractant after stripping, supporting its potential reuse, while the resulting lithium-rich solutions are compatible with conventional Li_2CO_3 production. Overall, although magnesium dominates organic-phase loading, calcium ultimately controls the operational window. These findings support a two-stage, native-pH strategy in which selective divalent-cation removal, particularly Ca management, conditions multicomponent Andean brines for subsequent efficient lithium recovery.

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Energy Balance and Technological Upgrade of an Anaerobic Digester Prototyping System for Biogas Production

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Biogas is a gaseous product derived from the anaerobic digestion of organic matter. Optimal production and the study of material interactions within this environment require digesters that precisely control process conditions, such as temperature and mixing [1]. This work documents the technological upgrade and energy balance of an anaerobic digester prototype, which works as a controlled testbed for evaluating the degradation of the Organic Fraction of the Urban Solid Waste [2]. The system is divided into four subsystems: an anaerobic reactor, a mixing tank, a solar heating unit used as thermal energy source, and a data acquisition system.

Recent modifications implemented to reactivate and optimize the prototype are detailed. These include the development of a custom single-layer Printed Circuit Board (PCB) for the DAQ, the installation of surface sensors in the solar collectors, and a highly precise capture and control software utilizing an Arduino Mega platform to regulate biomass heating and recirculation.

Commissioning tests using water as the working fluid quantified the energy transfer between the solar collectors and the digester through a heat exchanger. The energy balance of the overall system is presented, providing critical baseline operational data for both expected biogas production and future material degradation assays under the conditions reported in the original design. [3]

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CROSSLINKED ALGINATE-CLAY HYBRID BEADS FOR SUSTAINABLE CROP PRODUCTION

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The inefficient use of conventional fertilizers leads to severe nitrogen and phosphorus leaching [1]. To address this challenge, we developed a high-performance controlled-release fertilizer (CRF) based on Mg–Al hydrotalcites (HTs) intercalated with nitrate (HT-N) and phosphate (HT-P) via ultrasound-assisted coprecipitation (Mg/Al = 2:1), encapsulated in 2 wt.% calcium alginate beads [2]. XRD confirmed successful anionic incorporation with a $d_{(003)}$ interlayer distances of 9.03 Å and 9.23 Å for HT-N and HT-P, respectively, preserving the host clay's crystal structure during encapsulation [3]. Alginate spherification mitigated the initial burst release, turning an instantaneous release into a sustained, diffusion-controlled transport. Fitting to a semi-physical mathematical model decoupled intrinsic ion-exchange from matrix diffusion. Nitrates exhibited effective diffusivities (D_{eff}) of 7.31 to 7.53 x 10^{-11} dm^2/min, while phosphates released more slowly (D_{eff} of 3.42 to 3.51 x 10^{-11} dm^2/min) due to higher valence and matrix affinity [4]. Furthermore, 14-week soil column tests under systematic irrigation demonstrated that the hybrid beads sustained nutrient release, maintained high residual soil conductivity (6.68 mS/cm vs. 4.71 mS/cm for commercial fertilizer), and successfully buffered leachate pH within the optimal agricultural range of 6.5–6.8, preventing the severe soil acidification (pH ~ 5.3) induced by conventional ammonium nitrate. These results demonstrate that crosslinked alginate/hydrotalcite hybrid beads represent an efficient, sustainable, and economically viable technology for precision macronutrient management.

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From Plastic Waste to Advanced Materials: A Strategy for the Generation of Carbonaceous Structures.

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Carbon fiber is a high-performance material that plays an important role in the automotive industry due to its mechanical strength and light weight—essential attributes for reducing vehicle weight. Currently, more than 90% of the fibers available on the market are derived from polyacrylonitrile (PAN), a precursor that significantly increases production costs and limits its widespread use [1]. At the same time, the accumulation of polyolefin plastics, such as polypropylene (PP), poses a serious environmental challenge due to their lack of biodegradability. The purpose of this study is to develop an alternative and sustainable method for producing carbon fibers using polypropylene waste as a precursor, through a pyrolysis process.

To ensure the structural stability of the material and prevent the polypropylene from melting prematurely, the polypropylene fibers undergo a thermal and oxidative stabilization process to induce effective cross-linking of the polymer chains. Following this, the material is subjected to a pyrolysis process in an inert atmosphere [2]. Initial physicochemical characterization via X-ray diffraction confirmed that the precursor had a monoclinic phase, while thermogravimetric analysis helped determine the mass loss rates. The resulting fibers are expected to exhibit competitive properties for practical applications, thereby promoting recycling and the circular economy.

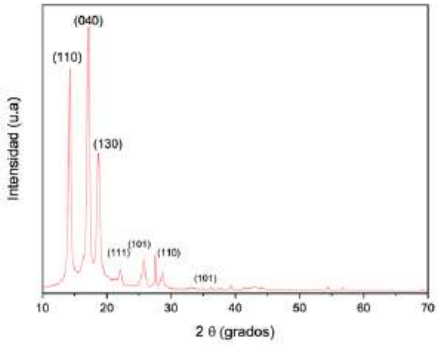

Figure 1. DRX PP

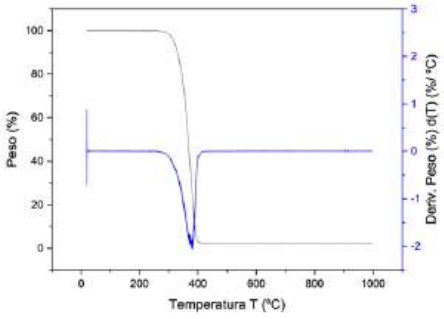

Figure 1. TGA PP

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FIRST-PRINCIPLES INVESTIGATION OF GLYCEROL ADSORPTION ON ALKALI BISMUTHATES: SURFACE REACTIVITY AND ELECTRONIC INTERACTION ANALYSIS

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The transition towards sustainable energy requires the industrial-scale valorization of biomass derivatives, such as glycerol, into clean energy carriers like hydrogen. While empirical approaches have demonstrated the catalytic efficacy of bismuth-based metal oxides for this purpose, fundamentally understanding their surface reactivity is imperative for the rational design and optimization of industrial catalysts. This work presents a comprehensive Density Functional Theory (DFT) study on the fundamental adsorption and cleavage mechanisms of glycerol over experimentally identified surfaces of $NaBiO_3$ and $LiBiO_2$. Adsorption energies and geometric interaction distances were systematically evaluated to identify the thermodynamically most favorable active sites. To elucidate the underlying electronic nature of the adsorbate-substrate interactions, charge transfer analyses were performed. Furthermore, Crystal Orbital Overlap Population (COOP) and Crystal Orbital Hamilton Population (COHP) partitioning schemes were employed to map the bonding and antibonding state populations. These analyses rigorously reveal the electronic mechanism dictating the catalytic weakening and subsequent cleavage of critical bonds within the glycerol molecule. By correlating experimental catalytic performance with quantum-mechanical descriptors, these theoretical findings provide a robust predictive framework for the mechanistic behavior of ternary metal oxides. Ultimately, this study underscores the critical role of first-principles modeling in accelerating the industrial deployment of advanced catalytic nanomaterials for green hydrogen production and environmental mitigation.

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Synthesis of magnetite nanoparticles coated with polyphenols towards development of biomedical applications

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Natural polyphenols are secondary metabolites with ring structures integrated by multiple substituent groups and hydroxyl (–OH) bonds. Due to the polyphenols properties including antioxidant, anti-inflammatory, anticancer, antibacterial, and anti-aging. These have potential applications in the treatment of different diseases including metabolic, cardiovascular, diabetes, neurodegenerative, and cancer. In this work, we have combined the single magnetic domains alignment of magnetite (Fe_3O_4) nanoparticles coated with polyphenols. The organic surface acts like phyto-reductants and facilitates the nanoparticles for cellular uptaken. Different groups of magnetite Fe_3O_4 nanoparticles (<20nm) have been synthesized and coated from polyphenols extracts from fruits and spices by a modified Massart's co-precipitation route. Polyphenols have been bonding on the nanoparticles surface by Fe–OH. We have reported the addressable magnetic domains behavior with available hydroxyl linkers –OH. The polyphenol layer thickness was observed in a range of 2-5 nm. Immortalized brain microglia murine cell line BV-2, ATCC showed an increased denaturation process in cell membranes as well as organelles from Magnetic Hyperthermia (MHT) [1].

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Enhanced Ciprofloxacin Photodegradation over Rubidium-Modified $BiVO_4$ Prepared by a Facile One-Pot Hydrothermal Route

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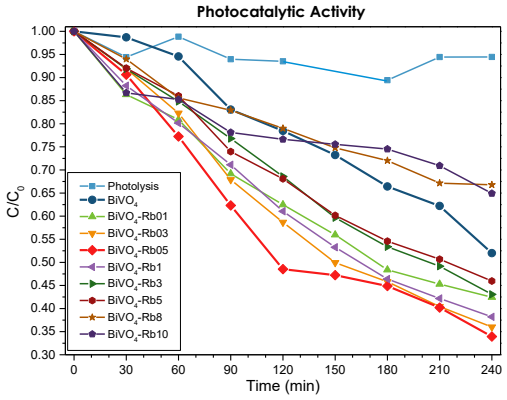
Nowadays water access is decreasing due to many factors as demographic explosion and water pollution. Among the principal water pollutants, there is the pharmaceutical compounds, e.i. ciprofloxacin, which after human consume, it is integrates to water as contaminant agent. This research is a contribution toward materials development for chemical compounds remotion. In this work, $BiVO_4$ chemically modified with Rubidium at different concentrations were synthetized by hydrothermal synthesis method. The present work aims to increment $BiVO_4$ photocatalytic properties. Catalysts powders were obtained in one-pot hydrothermal method, and characterized via X-Ray diffraction, Fourier-Transform Infrared spectroscopy, N_2 adsorption-desorption test and UV-Vis-NIR spectroscopy and X. As results, for concentrations of 0.5% and 1% Rb on $BiVO_4$, the photo-degradation of ciprofloxacin evaluated via UV-Vis spectroscopy reach to be more than 60% in 4 hours. The influence of synthesis parameters in the physical and chemical properties is discussed.



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Synthesis of Gadolinium-Doped Ceria (GDC) and Yttria-Stabilized Zirconia (YSZ) Thin Films for Solid Oxide Fuel Cell Electrolytes via the Pechini Method

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The growing demand for sustainable energy systems has driven the development of Intermediate Temperature Solid Oxide Fuel Cells (IT-SOFCs) to lower conventional operating temperatures, reducing interconnect costs and thermal degradation. This work focuses on the synthesis and characterization of gadolinium-doped ceria (GDC) and yttria-stabilized zirconia (YSZ) thin films for application as solid electrolytes. Materials were prepared via the Pechini sol-gel route, utilizing ethanol to ensure optimal wettability. To mitigate coefficient of thermal expansion (CTE) mismatches and prevent cracking, titanium substrates underwent sandblasting and chemical etching with oxalic acid. Additionally, YSZ required a controlled thermal pretreatment to release corrosive HCl gases prior to final calcination [1].

Structural characterization via XRD confirmed a crystalline, pure cubic fluorite phase. SEM and EDS analyses of the powders revealed porous, nanostructured fiber agglomerates with chemical purity and an absence of residual carbon. UV-Vis-NIR spectroscopy was used to calculate the optical bandgaps, highlighting the structural influence of the substrate.

Results show that combining pretreated titanium substrates, ethanol solvent, brush coating, and gradual heat treatment yields highly adherent, crack-free GDC and YSZ thin films. This scalable chemical route ensures their technical viability as efficient IT-SOFC solid electrolytes. Crucially for the industrial sector, replacing expensive high-vacuum deposition with this accessible methodology drastically reduces manufacturing costs and material waste, offering a highly profitable, sustainable, and ready to deploy solution for large-scale energy technologies [2].

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Characterization and degradation behavior of PLA fibers prepared by air-jet spinning

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In materials science, the synthesis method to obtain a material is very important, since it defines the main characteristics of the material. For polymers, their degradation under certain conditions not only defines their properties, but also their application. This work aimed to analyze the degradation of polylactic acid fibers synthesized by air-jet spinning (AJS) as possible scaffolds. The fibers' size was controlled through the PLA concentration, 6, 7, and 10 wt %. The morphology of the fibers spun was homogeneous, and the mean diameter sizes obtained were 600, 800, and 1400 nm, respectively. The initial crystallinity of the PLA turned into an amorphous phase after the stretching process by AJS. Degradation test by immersion of the fiber spun into bi-distilled water at different pH (5, 8, and 11) under a controlled CO_2 atmosphere at 36 ºC, showed excellent stability of the polymeric structure onto PLA fibers at 1, 3, 5 7, 14, and 21 days. Infrared spectra of the fibers under degradation do not present the band of COO^- group; it means that it does not exist an early degradation by hydrolysis of the PLA fiber spun, only a dissolution in the polymer chains is observed due to the pH changes presented in the solution at the end of the hydrolytic degradation test.

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NiO nanoparticles catalyst for the hydrogen evolution reaction

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In this study, nickel oxide nanoparticles (NiO NPs) were synthesized via the sol-gel method, with a focus on evaluating the influence of pH on crystal growth and particle size. After determining the optimal synthesis conditions, the physical properties of the NiO NPs were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). High-resolution TEM analysis revealed nanostructures with an average diameter of 50 ± 5 nm, while XRD confirmed high crystallinity, which can enhance charge transfer and increase the number of active sites for the hydrogen evolution reaction (HER) [1]. To assess their electrocatalytic performance, NiO NPs were incorporated into a catalyst ink prepared using deionized water, isopropanol, and Nafion®. The ink was then deposited onto a glassy carbon electrode (GCE) and dried at room temperature for 30 s. Electrochemical characterization demonstrated an overpotential of 690 mV and a Tafel slope of 173 mV dec^{-1} at 10 mA cm^{-2} (Figure 1), values comparable to benchmark catalysts [3]. These results suggest that NiO NPs are a promising, low-cost alternative to noble metal-based electrocatalysts.

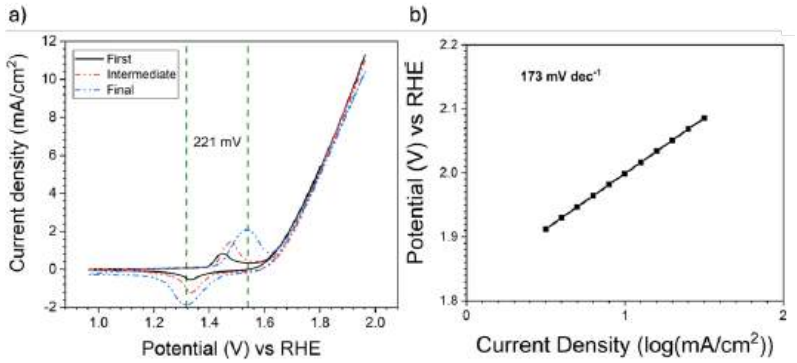

Figure 1.a) CV curve for NiO electrode at 10 mV/s and b) Tafel Plot

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HAFNIUM OXIDE NANOSTRUCTURES FOR NEXT GENERATION APPLICATIONS IN OPTOELECTRONIC DEVICES

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Hafnium oxide (HfO2)-based materials have been considered one of the most promising high dielectric constant (k=25) dielectrics for replacing silicon oxide (SiO2, k=5) in Complementary Metal-Oxide Semiconductor (CMOS) transistor fabrication technology. The eventual replacement of conventional low dielectric constant dielectrics in electronic and optoelectronic devices with hafnium oxide has led to an increased trend toward miniaturization of electronic devices, while preserving the insulating characteristics of their MOS structures and thus maintaining minimal leakage currents. [1-8] Hafnium oxide is characterized by a wide band gap (~5.8 eV), high transparency in the ultraviolet-visible spectral range, and a refractive index between 1.9 and 2.2. These properties open up a wide range of optical and optoelectronic applications, making this material particularly attractive for doping with rare-earth elements to exploit its luminescent properties in optoelectronic applications. [1-9] Luminescent materials are a field of study of interest for optoelectronic applications. Often called phosphors, these solids convert certain types of energy into electromagnetic radiation, rather than thermal radiation. Therefore, obtaining firsthand information on the optical and structural properties of hafnium oxide thin films doped with rare-earth elements is valuable work for considering their use in optoelectronic applications. [13] The uses of hafnium oxide have been documented in numerous works related to the fabrication of more efficient memories, MOSFET transistors with higher input impedance and lower leakage current, and capacitors with higher capacitance, among others. However, there is a lack of extensive literature related to the doping of this material with rare earth elements, resulting in limited applications in optoelectronics. [1,3,4,8]

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Abstract preparation

EFFECTIVE HEAVY LIQUID PRE-CONCENTRATION FOR THE ANALYSIS OF GOLD TELLURIDE MINERALS

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The presence of gold tellurides in refractory ores presents significant metallurgical challenges, requiring precise mineralogical characterization to properly identify the amount of gold and the correct treatment for gold extraction from the ores. In nature, gold tellurides are the most common form of chemical compound that gold forms due to the semi-metallic nature of tellurium and it can be present in different forms such as calaverite ($AuTe_2$), sylvanite [$(Ag,Au)_2Te_4$], krennerite [$(Au_{1-x},Ag_x)Te_2$] among others [1]. However, direct analytical observation without any pre-concentration is frequently hindered by the characteristically low grade and fine dissemination of these precious metal-bearing minerals within the host rock matrix (≈1gr Au /ton). To solve these limitations in gold analysis in laboratory conditions, a pre-concentration methodology utilizing heavy liquid separation was employed. This technique effectively isolated the high-density mineral fractions using tetrabromoethane (ρ=2.97 g/cm^3), significantly increasing the relative abundance of the target gold and telluride phases and eliminating the siliceous gangue and other relatively light particles.

The obtained heavy liquid concentrates were analyzed using Scanning Electron Microscopy along with Energy Dispersive X-Ray Spectroscopy (SEM-EDS). Within the concentrates, the SEM-EDS analysis yielded clear morphological and chemical identification of the gold and telluride mineral phases. This targeted characterization approach along with detailed elemental mapping allowed for the accurate determination of chemical associations between gold and telluride in industrial ores, providing critical qualitative and semi-quantitative data that would be unattainable in bulk sample analysis. The integration of density-based pre-concentration with advanced electron microscopy proves to be a highly effective diagnostic strategy for the mineralogical analysis of refractory gold ores.

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Evaluation of a Multicompartment Reactor for the Treatment of Secondary Sources of Base Metals

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The recovery of metals from secondary sources represents an alternative for supplementing the supply of raw materials and promoting their reintegration into the production cycle. The combinations of metals present in products considered as secondary sources often differ from those found in primary mineral deposits, posing new technological challenges for their efficient recovery. In favorable cases, such as the recycling of gold, silver, copper, lead, aluminum, and iron, high recovery efficiencies have been achieved. [1] [2]. However, in most cases, metal concentrations may be very low, or the combinations and proportions of metals may be unfavorable for processing, imposing both economic and technical limitations and highlighting considerable potential for process optimization. Although each metal could, in principle, be recovered separately, the mixture of different substances within a material stream poses significant challenges for metallurgical recovery. As the complexity of the mixture increases, metallurgical processing becomes more difficult and unavoidable metal losses tend to increase. Consequently, advanced metallurgical processes are required for the efficient recovery of technologically valuable metals from complex materials.

In the present work, a combined hydrometallurgical process involving solvent extraction and facilitated transport through an electromembrane system was evaluated for metal recovery from synthetic multicomponent solutions designed to simulate those potentially generated during the treatment of secondary sources containing Cu, Ag, Pb, Zn, Fe, and Ni. The proposed process consists of a reactor with three compartments—feed, membrane, and stripping—which is electro-assisted to enhance ionic transport. Within the membrane compartment, the selective extraction of metallic species is promoted using a synthetic resin impregnated with a D2EHPA–kerosene extractant solution. The results showed the effectiveness of the selective separation of metal ions, as evidenced by differences in the transport and distribution of the species among the different reactor compartments. The combination of extraction and electro-assisted transport enabled the evaluation of the system's ability to selectively concentrate metal species from a multicomponent matrix, providing an alternative approach for their subsequent recovery. Furthermore, operation under moderate conditions and the relatively low consumption of reagents and energy highlight the potential of this process for integration into hydrometallurgical routes aimed at the valorization of secondary sources.

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In situ functionalization of nanoparticles with clove polyphenols via the co-precipitation method.

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Superparamagnetic iron oxide nanoparticles (SPIONs) find extensive applications across biomedical, technological, and industrial sectors, owing to their tunable magnetic properties which depend on size, shape, composition, and surface characteristics. Precise control over their synthesis and properties is crucial for evaluating their performance and potential environmental or health risks.

In this study, manganese ferrite ($MnFe_2O_4$) were synthesized via co-precipitation using iron and manganese chloride precursors. The process involved 30% HCl diluted in distilled water, with argon gas used for solvent degassing. KOH served as the precipitating agent, added to the chloride solution at a specific molar ratio. Finally, the nanoparticles were functionalized with a clove extract solution to enhance their biological affinity with Fe/Mn-OH bonding over nanoparticles surface.

The physical properties of the $MnFe_2O_4$ nanoparticles, including size distribution and elemental composition, were analyzed via SEM-EDS. Structural characterization was performed using XRD and SAED, while TEM was employed to observe morphology and the polyphenol coating. Additionally, FTIR spectroscopy was used to identify the chemical composition and primary functional bonds within the nanoparticles.

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Session 5. Coordination Compounds

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Pd(II) AND Ag(I) COMPLEXES WITH PYRAZOLHYDRAZIDE-HYDRAZONE LIGAND: *IN VITRO* ANTIMICROBIAL ACTIVITY AGAINST *S. AUREUS* AND *E. COLI*

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In this work, the *in vitro* antimicrobial activity against *S. aureus* and *E. coli* was evaluated using the agar well diffusion method [1] for palladium(II) (**C1**) and silver(I) (**C2**) complexes, obtained from the hydrazide-hydrazone ligand (**L**) and pyridine (py) as a coligand. Ligand **L** was synthesized by the condensation reaction between 1,3-diphenylpyrazol-4-carbaldehyde and 4-hydroxybenzohydrazide, under reflux for 24 h. Complexes **C1** and **C2** were prepared in acetone from a stoichiometric mixture of ligand **L**, pyridine (py), and the corresponding metal salts, under constant stirring for 3 h.

The structural characterization of **C1** and **C2** was carried out by comparing the IR spectra of the free ligand with those of its corresponding complexes, which allowed the formation of the compounds [Pd(**L**)(OAc)(py)] and [Ag(**L**)$(py)_2$]NO_3 to be proposed. It was observed that ligand **L** coordinates to the metal center in a bidentate manner, acting as an enolate tautomer in the Pd(II) complex and as a keto tautomer in the Ag(I) complex through the carbonyl oxygen and azomethine nitrogen donor atoms. The proposed structures were confirmed by the absence of the absorption band attributed to $\nu(C{=}O_{amide})$ in the spectrum of **C1**, the shift of this band from 1651 to 1628 cm^{-1} in **C2**, and the shift of the band associated with $\nu(–CH{=}N–)$ from 1551 cm^{-1} in **L** to 1535 cm^{-1} and 1543 cm^{-1} in **C1** and **C2**, respectively. Elemental analysis (CHN), melting point determination, and other complementary analytical techniques confirmed the purity and composition of the synthesized compounds.

The results showed that **C2**, dissolved in DMSO, exhibited the highest antibacterial activity, with a minimum inhibitory concentration (MIC) of 0.05 $mg{\cdot}mL^{-1}$, compared with the values obtained for **L** and **C1** (5 $mg{\cdot}mL^{-1}$). The remarkable activity of the silver(I) complex may be attributed to the ability of the azomethine group (–CH=N–) to establish hydrogen bonding interactions with biomolecules in the cellular environment, as well as to the synergistic effect of pyridine (py) as a coligand, which would promote the permeability of Ag(I) ions and alter essential cellular processes [2].

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SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL EVALUATION OF IMINO PHOSPHINE P-N Pd(II) COMPLEXES DERIVED FROM SCHIFF BASES

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The rising incidence of bacterial infections resistant to conventional antibiotics constitutes one of the primary global public health challenges. Antimicrobial resistance has become critically relevant as numerous infections no longer respond to available therapies. This crisis has driven the search for novel treatments and therapeutic strategies based on compounds with alternative mechanisms of action, among which metal complexes stand out due to their structural versatility and potential biological activity. Coordination complexes represent a strategic platform for developing new therapeutic agents, allowing for the rational modulation of both physicochemical properties and biological activity through the precise selection of metals and ligands [1]. The incorporation of Schiff bases as ligands offers additional advantages by enhancing complex stability and promoting interactions with relevant biological systems. In this context, the present work focuses on the design, synthesis, and characterization of new metal complexes derived from Schiff bases [2,3]. A series of imino-phosphine P-N Pd(II) complexes was synthesized using various aliphatic amines. Minimum inhibitory concentrations (MICs) and minimum fungicidal concentrations (MFCs) were determined against several Gram-positive and Gram-negative bacterial strains, as well as *Candida* species. Among the evaluated compounds, complex 3 exhibited the highest antimicrobial activity, demonstrating both bactericidal and fungicidal effects. Overall, these results highlight the promising therapeutic potential of imino-phosphine P-N Pd(II) complexes as multifunctional candidates with both anticancer and antimicrobial properties.

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SYNTHESIS, STRUCTURAL DETERMINATION AND TD-DFT CALCULATIONS OF A SERIES OF *N*-NAPHTYL(ETHYLENE)IMINES AND THEIR ZINC COMPLEXES

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Neglected diseases predominate in tropical and subtropical nations, proving to be a significant public health problem. Trypanosomiasis[1] and leishmaniasis[2] represent two major neglected diseases widespread in southern Mexico. There is an urgent need to develop new anti-kinetoplastids agents that exhibit lower toxicity and greater activity. Polyamine (and imine) derivatives have been evaluated as promising antitrypanosomal and antileishmanial agents. The use of *N,N*-disubstituted diamines based on putrescine and 1,3-propanediamine fragments with aliphatic chains that exhibited sub-micromolar activity in the treatment of leishmaniasis and trypanosomiasis. [3-5] Coordination complexes of polyamines and imines with various metal ions have been evaluated as anti-kinetoplastid agents, particularly with Zn,[6] with some complexes inhibiting, for example, the Fe-SOD complex. Herein, we report the synthesis of a series of *N*-(Naphthyl)ethylenediimine ligands using pyridine motifs, and their Zn complexes, with DFT calculations for the structure analysis in the excited state. The NMR analysis shows distinctive chemical shifts for the pyridine structure alongside the ethylenediamine linker as two *dd* in the aliphatic region. TD-DFT analysis using the CAM-B3LYP/6-311G(d,p)/6-311+G(d,p) level of theory, applied to the gas-phase optimized structures, reveals that the first excited-state transition in compounds L1–L3 involves of combinations of transitions. NCI analysis of the non-covalent interactions shows a weak interaction between the imine nitrogen and the NH hydrogen. When reaction of Zn halide salts with each of the three ligands, NMR analysis shows that the NH fragment of the amines coordinates to the metal ion due to upfield chemical shift of the signal.

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Abstract preparation

Espectrometría de Absorción Atómica de Fuente Continua (HR-CS AAS). Trazabilidad Multielemental Ultrafina y Caracterización Elemental de Nuevos Materiales.

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La caracterización de materiales avanzados demanda un equilibrio riguroso entre precisión analítica y eficiencia operativa en entornos de I+D. La Espectrometría de Absorción Atómica de Fuente Continua de Alta Resolución (HR-CS AAS), representada por la serie *contrAA* de Analytik Jena, supera las limitaciones del análisis monoelemental convencional mediante el empleo de una única fuente de radiación de arco corto de xenón. Este principio físico-químico otorga acceso ininterrumpido a todo el espectro óptico atómico y molecular, posibilitando el análisis multielemental secuencial rápido en matrices complejas como nanoestructuras, polímeros dopados y aleaciones especiales, con la consecuente optimización de costos y plazos de desarrollo.

El fundamento del sistema reside en su acoplamiento óptico de un monocromador Echelle de alta resolución con un detector CCD lineal, combinación que permite la resolución y corrección tridimensional de interferencias de fondo en tiempo real a escala picométrica. En términos metrológicos y comerciales, la plataforma alcanza límites de detección en el rango de sub-ppb a ppb, ofreciendo una fiabilidad equivalente a técnicas multielementales complejas como ICP-OES, pero con menor costo de infraestructura y la flexibilidad de alternar de forma automatizada entre atomización por llama, horno de grafito e hidruros. De este modo, la tecnología HR-CS AAS consolida la precisión de laboratorio como una ventaja competitiva en la innovación de materiales de nueva generación.

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TUNING Tb(III) LUMINESCENCE USING 2-SUBSTITUTED PNC-TYPE ANTENNA LIGANDS

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Tb(III) complexes are attractive green emitters, but their parity-forbidden f–f transitions have very low molar absorptivities, therefore an organic chromophore is required to sensitize them through the antenna effect. PNC or CAPhs ligands are appealing antennas: their C=O and P=O donors form robust chelates, which are easily tuned electronically by substitution. In this work, a family of four proligands of general formula $(PhC_4H_8N)_2P(O)NHC(O)C_6H_4$-2R (LH-R) with R= H (1), Me (2), Cl (3) and NO_2 (4) were prepared through an optimized three-step route in yields of up to 83%, and coordinated to Y^{3+}, La^{3+} and Tb^{3+} to afford twelve tris-chelate complexes of general formula $Ln(L\text{-}R)_3 \bullet nH_2O$.

All compounds were characterized by multinuclear NMR (^1H, ^{13}C, $^{31}P\{^1H\}$), ESI and DART mass spectrometry, FTIR-ATR, elemental analysis and TGA/DSC. Single-crystal X-ray diffraction of the proligands revealed dimers assembled through N–H···O=P hydrogen bonds. Complex IR-spectroscopy confirmed bidentate coordination through the carbonyl and phosphoryl groups, thermal analyses showed the presence of two to four water molecules per complex and demonstrated that the complexes are thermally stable up to ca. 300 °C.$^{31}P\{^1H\}$ NMR evidenced an equilibrium in solution between coordinated and free ligand.

Photophysical studies in $CHCl_2$ and toluene gave molar absorptivities in the 10^3–10^4 M^{-1} cm^{-1} range. The $Tb(L\text{-}R)_3$ (R = H, Me, Cl) complexes exhibit bright green luminescence in solution and in the solid state, with the full set of $^5D_4 \rightarrow {}^7F_j$ (J = 6–0) transitions, emission lifetimes of 1.3–1.5 ms and absolute solid-state quantum yields between 20.6–43.5%, the highest value corresponding to the electron-donating methyl derivative. In contrast, $Tb(L\text{-}NO_2)_3$ is essentially non-emissive (Φ = 0.22%), which is ascribed to the strongly electron-withdrawing nitro group lowering the ligand triplet state below the level required for efficient energy transfer to Tb(III). Substituent tuning of PNC antennas are therefore effective handle for controlling Tb(III) sensitization, and these complexes are promising candidates for optical materials [1–3].

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Mono-, Bis- and Tris(dimethylamide)Titanium(IV) Complexes: Synthesis, Characterization and CO_2 Reactivity

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Diamides are versatile ligands widely used in nuclear waste treatment to recover lanthanides and actinides (e.g., the DIAMEX process) [1]. However, the influence of substituents on their basicity and coordination behavior remains understudied. In this work, the divergent reactivity of amides H_2DMDMMA and H_2DTDMMA toward $Ti(NMe_2)_4$ is presented [2]. This approach provides a systematic collection of titanium(IV) amide–malonate complexes displaying remarkable structural diversity, including species bearing one, two, or three dimethylamide groups and distinct *cis*-OO′ and unprecedented *cis*-NO coordination modes (**Figure 1**). Under mild conditions, these complexes react with CO_2, resulting in titanium(IV) carbamate complexes. The findings provide an insight into the relationship between ligand basicity and coordination mode.

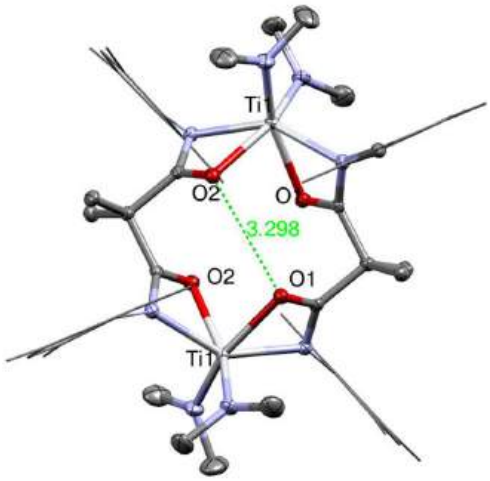

Figure 1. Molecular structure for *cis*-NO titanium amide malonamide with thermal ellipsoids at 50% probability. Hydrogen atoms are omitted for clarity. Mesityl groups are displayed as wireframes.

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COORDINATION GEOMETRIES AND ARGENTOPHILIC INTERACTION INDUCED BY THE TRIPYRIDYLIMIDAZOLINE LIGAND IN A DINUCLEAR Ag(I) COMPLEX: STRUCTURAL ANALYSIS AND DFT STUDIES

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Silver(I) coordination complexes have attracted increasing attention due to their structural diversity and the flexible coordination behavior of the d^{10} Ag(I) center. These characteristics support their use in luminescent materials, antibiotic development, and catalytic applications. [1]. In particular, short Ag•••Ag contacts associated with argentophilic interactions represent an important structural feature in polynuclear silver(I) systems and can contribute to their molecular organization [2]. In this study, a dinuclear Ag(I) complex based on *cis*-2,4,5-tris(pyridin-2-yl)imidazoline (**L**) and *p*-toluenesulfonate ($\mathbf{OTs^-}$) was synthesized and characterized using complementary experimental and computational methods. Infrared analysis showed shifts in the characteristic C=N and N–H stretching vibrations upon complex formation, along with characteristic bands of the OTs^- anion [1, 2]. Single-crystal X-ray diffraction analysis showed that the complex crystallizes as a dinuclear cationic unit, $\mathbf{[Ag_2(L)_2(OTs)]^+}$. The structure consists of two crystallographically independent Ag(I) centers with distinct coordination environments. Ag(1) exhibits a highly distorted four-coordinate environment, whereas Ag(2) is five-coordinate and adopts a distorted trigonal-bipyramidal geometry, with an oxygen atom from a coordinated OTs^- anion completing its coordination sphere. The Ag(1)•••Ag(2) separation of 2.999(4) Å is consistent with an intramolecular argentophilic interaction. DFT optimization showed a 96% structural similarity between the calculated geometry and the experimental crystal structure, supporting the consistency of the computational model. TD-DFT calculations reproduced the main absorption region of the experimental UV-Vis spectrum, with minor shifts in band positions. Hirshfeld surface analysis showed that H•••H, H•••O/O•••H, and C•••H/H•••C contacts represent the main contributions to the crystal packing, highlighting the role of hydrogen bonding and other weak intermolecular interactions in the supramolecular organization of the complex. This work contributes to the study of dinuclear Ag(I) architectures and to a better understanding of their structural, supramolecular, and electronic features.

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AMINO ACID-BASED LIGANDS AS VERSATILE PLATFORMS FOR POLYMERIC COORDINATION COMPOUNDS: FROM STRUCTURE TO POTENTIAL APPLICATIONS

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Amino acids are readily available, enantiomerically pure chiral building blocks. Due to the presence of amino and carboxylate functionalities, they act as highly versatile ligands for the synthesis of chiral coordination compounds. Moreover, straightforward derivatization further expands their structural diversity, making them particularly attractive platforms for ligand design. The combination of intrinsic functional groups and tailored modifications enables efficient and directional intermolecular interactions, especially hydrogen bonding, promoting the formation of robust crystalline materials with rich supramolecular architectures. Beyond structural interest, amino acid- and peptide-based materials have attracted considerable attention for biomedical applications and as sustainable alternatives to conventional synthetic systems [1].

In this talk, I will present recent results from our group on several ligand families derived from the reaction of the amino acids L-Alanine (Ala), L-Aspartic acid (Asp), L/D-Phenylalanine (Phe) and L/D-Tyrosine (Tyr) with different aldehydes. These compounds serve as versatile ligands for the construction of a broad range of coordination architectures. Depending on the ligand structure, metal ion, and reaction conditions, the resulting assemblies include mononuclear complexes, trinuclear species, and one-, two-, and three-dimensional coordination polymers exhibiting diverse structural features. One of the main challenges in the study of these systems is elucidating the structure–property relationships and the influence of supramolecular chemistry [2, 3]. For instance, alanine-derived ligands have so far yielded exclusively mononuclear complexes, whereas phenylalanine- and tyrosine-based systems can generate extended coordination polymers, highlighting the influence of side-chain functionality. In addition, the use of first-row transition metals combined with amino acid-based ligands provides access to systems with potential biorelevance and biocompatibility. Regarding potential applications, selected Cu^{2+} complexes have been evaluated as nitrite reductase mimics [3], while Cu^{2+}, Co^{2+} and Cd^{2+} coordination polymers have shown catalytic activity in the aerobic oxidation of cycloalkenes under mild, environmentally friendly conditions (low temperature, atmospheric pressure, solvent-free) [4]. The use of L- and D-amino acids enables the preparation of enantiomeric compounds, opening the door to studies of enantioselective behavior. In addition, a Mn^{2+} one-dimensional coordination polymer is currently under investigation as a potential magnetic resonance imaging (MRI) contrast agent, with promising preliminary results.

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Synthesis, Characterization, and Evaluation of the Antidiabetic Activity of Zinc Complexes with Schiff Base Ligands Derived from L-Phenylalanine

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En este trabajo se realiza la síntesis y caracterización estructural de nuevos complejos de zinc con ligantes tipo base de Schiff derivados de L-fenilalanina como aminoácido, y 2-hidroaxiacetofenona y 5-cloro-2-hidroxiacetofenona; con el objetivo de explorar su potencial como candidatos terapéuticos frente a la Diabetes Mellitus Tipo 2. La caracterización de los ligantes y sus complejos de zinc se realizó mediante la espectroscopia de infrarrojo (IR9, ultravioleta visible (UV-Vis) y la determinación del punto de fusión. Se confirma la coordinación metal-ligante mediante estudios espectroscópicos y fisicoquímicos. Estos resultados constituyen la base para investigaciones posteriores enfocados en la evaluación de su potencial actividad antidiabética, particularmente en la inhibición enzimática y en modelos experimentales.

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IMINOBENZOCALCOGENAZOLYL CALCOGENPHOSPHINATES: NEW PNC-TYPE LIGANDS FOR ELECTRON DENSITY ADDRESSING

Oscar Luis García-Guzmán[1], Verónica García-Montalvo[1*]

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Oxidation of the aminophosphines, $^{i}Pr_2PNHC(Y)NC_6H_4$ (Y = O (**1**) and Y = S (**2**)), yielded a new series of iminobenzoxazolyl and iminobenzothiazolyl PNC-type proligands, $^{i}Pr_2P(X)N{=}C(Y)NHC_6H_4$ with X = Y = O (**3**); X = S, Y = O (**4**); X = O, Y = S (**5**); X = Y = S (**6**) [1]. The corresponding zinc(II) PNC-type complexes, $[Zn\{^{i}Pr_2P(X)N{=}C(Y)NHC_6H_4\text{-}\kappa^2\text{-}X,N\}_2]$ with X = Y = O (**7**); X = S, Y = O (**8**); X = O, Y = S (**9**); X = Y = S (**10**), were obtained in good yields by ethane elimination reaction between $ZnEt_2$ and the corresponding proligand in toluene [2]. All the compounds were characterized by elemental analysis, multielement NMR, FTIR, UV-Vis spectroscopy, fluorimetry, and mass spectrometry. The eight compounds (**3**-**10**) were structurally charaterized by using single-crystal X-ray diffraction (SCXRD). The molecular structures of the proligands (**3**-**6**) showed a tautomeric arrangement with the acidic hydrogen on the endocyclic nitrogen (N_{endo}–H) in both solution and the solid state. SCXRD molecular structures of complexes (**7**-**10**) revealed bidentate ligands bonded to the metal center through the X and endocyclic N atoms (κ^2-*X*,N_{endo}) in a distorted tetrahedral coordination geometry around Zn(II). Notably, the ^{31}P- and $^{31}P\{^{1}H\}$-NMR spectra of (**1**) revealed an equilibrium between the P–H (hydrogen on phosphorus) and N_{exo}–H (hydrogen on the exocyclic nitrogen) tautomers, whereas while compound (**2**) exhibited the preferential formation of the N_{exo}–H (hydrogen on the exocyclic nitrogen) tautomer. Additionally, substituted iminobenzothiazolyl thiophosphinate proligands and their corresponding zinc(II) complexes were synthesized and characterized, $^{i}Pr_2P(S)N{=}C(S)NHC_6H_3Z$ and $[Zn\{^{i}Pr_2P(S)NC(S)NC_6H_3Z\text{-}\kappa^2\text{-}X,N\}_2]$ (Z = -6OEt, -6Me, -6Cl, -6NO_2, -4Me, -4Cl). These derivatives provide a systematic platform for investigating how variations in the chalcogen atom and substituent pattern modulate the electron density distribution within the metallacyclic framework and enable electron density addressing in Zn(II) complexes (*Figure 1*).

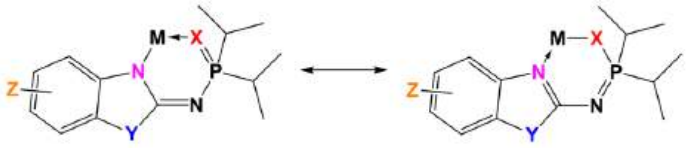

Figure 1

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Counterion-Programmed Capture or Conversion of SO_2 within a Pd_6L_8 Metal−Organic Cage

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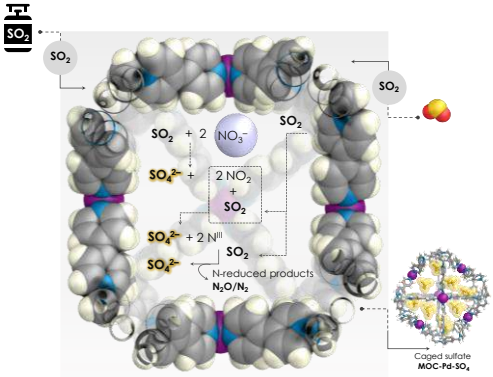
The continuous emission of harmful gases into the atmosphere damages the environment, air quality, and public health worldwide. Effective mitigation requires materials that both capture and inactivate these gases, yet integrating and precisely controlling these functions within a single system remains challenging. Here, we demonstrate for the first time that switching between SO_2-physisorption and chemisorption in porous materials can be achieved through counterion selection, as illustrated with cationic Pd_6L_8 Metal-Organic Cages (MOCs). MOCs with BF_4^-, PF_6^-, or SO_4^{2-} expressed reversible SO_2 uptake (up to 3.6 mmol g^{-1}), whereas NO_3^- promotes *in situ* oxidation to sulfate. The nitrate-bearing MOC captures 6.0 mmol g^{-1} of SO_2, converts it quantitatively to SO_4^{2-} within its cavity (94% yield, room temperature), and is fully regenerable—an unprecedented performance among SO_2 adsorbents. Thus, counterion-directed adsorption offers a programmable strategy for advanced gas remediation materials.



Schematic representation of the cavity-mediated mechanism of SO_2 to SO_4^{2-} transformation within a molecular cage.

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Developing a charge-and-shape mismatch strategy for the synthesis of porous weakly bonded frameworks based on coordination compounds or inorganic polyanions.

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Coordination compounds feature unique properties that allow them to serve as building blocks in supramolecular chemistry, providing geometries that are difficult to reproduce with organic building blocks, tunable charges, and adjustable rigidity. In this work, we present the case of UNAM-1, a hydrogen-bonded framework composed of a tridecanuclear copper coordination complex anion and dimethylammonium cations.[1] Although it is only sparingly soluble in most organic solvents, it can be solubilized in water and formamide, and such solutions can be used for cation exchange, conserving the anion's structure. Developing a charge-and-shape mismatch strategy, we replaced the dimethylammonium cation with the phenyl-1,4-diamidinium dication, resulting in the formation of UNAM-2, a more stable, hydrogen-bonded framework with a predictable structure and permanent porosity.[2] Finally, testing the limits of the charge-and-shape mismatch strategy, a flexible, ionic, and conductive compound, UNAM-3, was synthesized from a Keggin silicotungstate polyoxometalate tetraanion and tetraethylbenzidine radical cations.[3]

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Coordination compounds as molecular models of silica-supported single-site catalysts seen through quantum crystallography.

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Vojtech Jancik[1,2], Oscar Fernando López[1,2], Belén Sánchez Sánchez[1,2], Juan de Dios Guzmán Hernández[1,2], Diego Martínez Otero[1,2]

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Single-site catalysts supported on an inert material, such as silica, combine the ease of separation of heterogeneous catalysts with the maximum activity of homogeneous catalysts. However, this also contributes to the difficulties encountered during the study and characterization of these supported active sites, as their aleatory distribution and low concentration on the surface of the inert support significantly increase the experimental challenge. One possibility to overcome this problem is to develop molecular compounds that mimic the Si-OH groups on the silica surface and stabilize the same active site.[1–3] Therefore, we have designed several bulky silanols that were used to stabilize monomeric models of group-four amide species identified previously on modified silica surfaces. Herein, we present a quantum crystallographic analysis of the steric and electronic effects induced by the silanol ligands on the metal centers and the electron density distribution within different metallosilicate units.

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MAIN GROUP SUPRAMOLECULAR CHEMISTRY: FROM METALLOID-DIRECTED SELF-ASSEMBLY TO CYCLOPHANES

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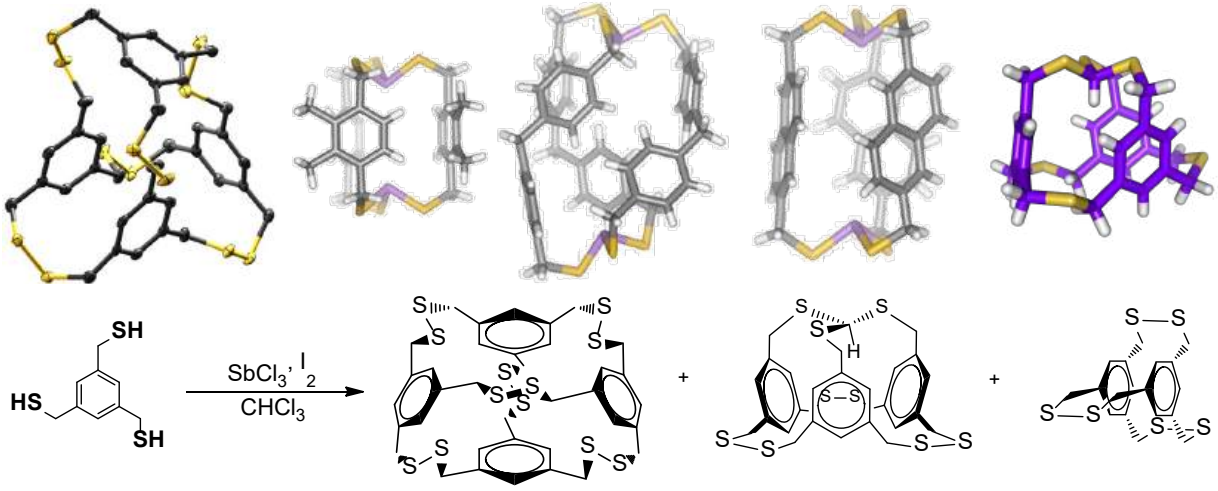
This talk will begin with a historical overview of our work in main group ion directed self-assembly to set the stage for current studies in disulfide self-assembly of cages and nanohoops. Reversible metal-ligand interactions have been used as an important tool to self-assemble numerous spectacular, discrete supramolecular structures. We previously developed a design strategy for using the unusual coordination chemistry of main group metalloid ions as directing elements in self–assembly reactions to form three-dimensional, multinuclear supramolecular assemblies. For example, the trigonal pyramidal coordination geometry of Group 15-thiolates leads to self-assembly of a series of E_2L_3 "cryptands" and macrocycles (E=As, Sb).[1]

These main group assemblies, while quite stable to air, moisture, acid and base, react cleanly with mild oxidizing agents to yield discrete disulfide macrocycles and cages.[2] This talk will describe the scope of this reactivity, showing that the process can efficiently prepare known and new cyclophanes, cages, and nanohoops in surprisingly efficient reactions directly from thiols under dynamic covalent control. Efforts to explore steric and electronic effects as well as the use of "self-sorting" to control self-assembly will also be discussed.[3]



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(Hf)PCN-224(Co) AS AN EFFICIENT PPM-LEVEL SENSOR FOR TOXIC SO_2

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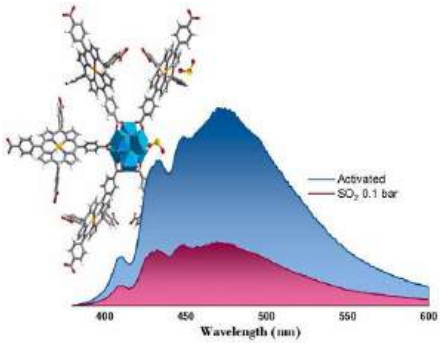
The highly porous hafnium cobalt-porphyrin tetracarboxylate named (Hf)PCN-224(Co) was used as fluorescent probe material to detect sulfur dioxide (SO_2). (Hf)PCN-224(Co) demonstrated a moderate SO_2 sorption of 1.0 mmol g^{-1} at 0.1 bar and 298 K, and a limit of detection of 175.5 ppm, obtained by photoluminescent experiments. Furthermore, clear, different emission responses are observed for (Hf)PCN-224(Co) after the exposure to CO_2 and water vapor, compared to SO_2. The use of Hf^{4+}, as well as microwave-assisted solvothermal synthesis, lead to crystalline defects in the form of missing linkers, providing additional Hf(IV) open metal sites, able to interact with SO_2 molecules. Based on UV–Vis and X-ray photoelectron spectroscopies, we suggest ligand to metal charge transfer as primal emission mechanisms, and the coordination of SO_2 with $Hf_6(OH)_8$ coordinatively unsaturated clusters as the most plausible origin for the emission response in SO_2 detection/sensing [1,2]. The tendency of this behavior is verified from the density functional theory calculations.



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WATER-SYNTHESIZED COORDINATION POLYMER USED IN HIGHLY REVERSIBLE ELECTRODE: FIRST ASSESSMENT OF CHARGE STORAGE PROPERTIES

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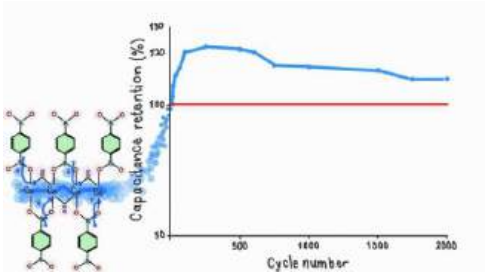
Herein, we established an eco-friendly method to synthesize a coordination polymer (CP) based on benzene-1,4-diboronic acid (BDBA) and Co(II) atoms, entitled Co-BDBA, using only water in the whole synthetic process. Co-BDBA is a crystalline material comprising a mesoporous structure with specific surface area and a mean pore size of 104.9 $m^2\ g^{-1}$ and 3.4 nm, respectively. Remarkably, Co-BDBA features enhanced electrochemical properties, especially in terms of electrochemical reversibility with a specific capacitance of 345 F g^{-1} at 1 A g^{-1} and superior capacitance retention of 109.7% after 2000 galvanostatic charge–discharge cycles. The voltammograms and the galvanostatic charge–discharge profiles indicate a pseudocapacitive behavior, where the energy storage kinetics is controlled by surface processes, *i.e.*, a capacitive-controlled energy storage kinetics, contrary to the majority of coordination polymers previously reported [1,2]. Finally, capacitive-controlled energy storage kinetics was also confirmed by electrochemical impedance spectroscopy experiments.



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SUPRAMOLECULAR CHEMISTRY ON NANOCARBONS FOR DISPERSIBILITY AND PHASE TRANSPORT

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Carbon nanostructures encompass a wide range of architectures and exhibit remarkable physicochemical properties, making them attractive for applications in catalysis [1], energy conversion and storage, sensing and diagnostics [2], as well as emerging biomedical technologies such as conductive tissue regeneration [3]. Their incorporation into nanocomposites is particularly promising for advanced materials, although achieving homogeneous dispersion and effective interactions with the surrounding matrix remains a major challenge. Non-covalent functionalization provides a versatile approach to address this issue while minimizing disruption of the intrinsic properties of the nanocarbons and facilitating their processing under different conditions. This lecture will present two supramolecular strategies being investigated in our labs.

The first approach relies on self-assembling tripeptides capable of adopting amphiphilic conformations. These molecules act as supramolecular surfactants, enabling the dispersion of nanocarbons in aqueous media, including solutions with high ionic strength. Beyond stable dispersions, this strategy also provides access to nanocomposite materials and supramolecular hydrogels. Particular attention has been devoted to the influence of morphology and nanoscale dimensions, as well as to the comparison between supramolecular assembly and covalent functionalization. These studies have helped identify the structural and interaction parameters governing the formation of self-healing hybrid materials [4].

The second strategy uses metal–organic cages, in which aromatic interactions are exploited to promote the dispersion of nanocarbons in polar solvents. By exchanging the cage counterions, this approach can additionally induce phase transfer between media. A key advantage of this method is the reversible nature of the functionalization: when required by the target application, the cages can be readily disassembled and separated from the nanocarbon surface [5].

Together, these examples illustrate how supramolecular chemistry can provide adaptable and reversible tools for controlling the processing and organization of carbon nanostructures, while retaining their desirable properties for incorporation into advanced functional materials.

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AN UNUSUALLY ACIDIC METHYL GROUP

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Coumarins featuring A–π–D push–pull systems often exhibit excellent electronic properties associated with strong intramolecular charge transfer (ICT).[1] Characterization of the 3-acetyl-7-(diethylamino)-4-hydroxy-2H-chromen-2-one (HC7A) molecule revealed unusual spectroscopic and acid–base properties.[2] In this work, its behaviour was further investigated by ^{1}H NMR and UV–Vis absorption spectroscopy upon MeONa addition, and by fluorescence emission spectroscopy in different solvents (EtOH, MeOH, toluene, $CHCl_3$, MeCN, and CH_2Cl_2).

Addition of multiple equivalents of MeONa to HC7A in MeOH resulted in a decrease of the main UV–Vis absorption band at 388 nm and the emergence of a higher-energy band at 342–345 nm. ^{1}H NMR analysis in CD_3OD revealed deuterium coupling of the acetyl $-CH_3$ signal upon base addition. Fluorescence measurements revealed a pronounced solvent dependence.

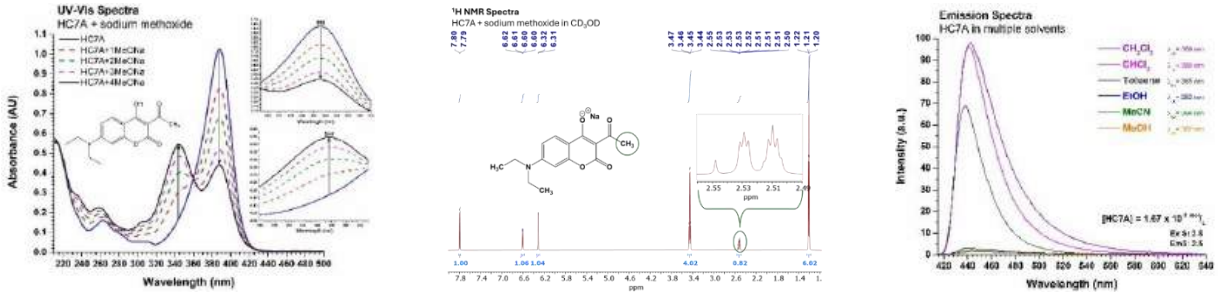

Fig 1-3 HC7A+MeONa UV-Vis Spectra (left) and ^{1}H NMR Spectra (center). HC7A fluorescence spectra in multiple solvents (right).

The incorporation of 7-diethylamino, 3-acetyl, and 4-hydroxy substituents imparts the coumarin with diverse absorption, emission, and acid–base properties, suggesting its potential as an antenna ligand in lanthanide coordination compounds.[3, 4]

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Substituent-Controlled Solubility and Structural Adaptability in 3d-Metal Chalcogenophosphinoyl Metallascorpionates

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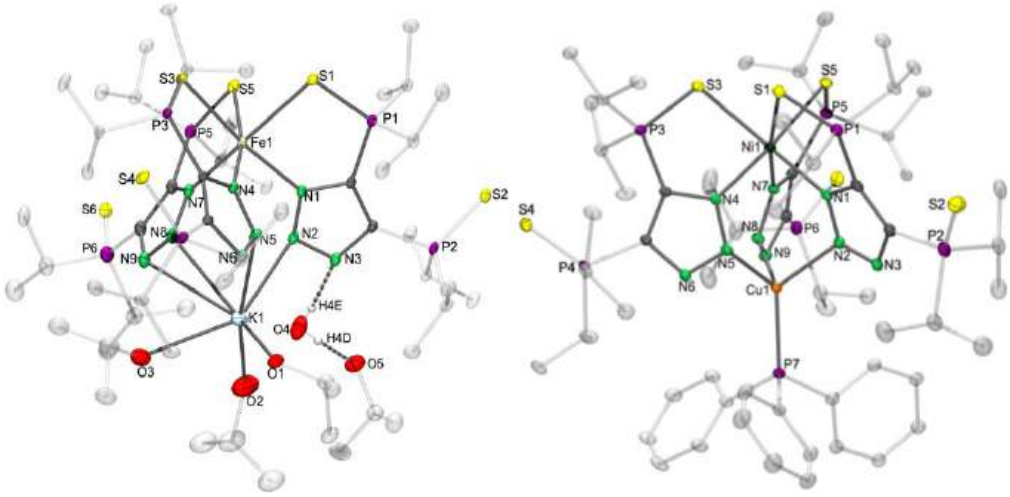
Chalcogenophosphinoyl triazolates provide a versatile platform for the metal-directed self-assembly of 3d-metal metallascorpionates and the construction of heterometallic architectures [1]. The effect replacing the groups at phosphorus in sulfur-containing triazolates was studied in self-assembly reactions with Zn, Co(II), Ni(II), Fe(II), and Mn(II) producing stable M/K metallascorpionate arrangements. The isopropyl groups improve solubility while perserving the metallascorpionate moiety. These systemas are also stable in air and can be crystallized from solvent mixtures containing isopropanol and water. Structural comparison in the solid-state structures shows moderate effect on the immediate coordination environment of the transition metal, but produce more noticeable changes in the M···K separation and in the geometry of the outer potassium-containing region. Furthermore, theses M/K metallascorpionates are useful synthons in metathesis reactions leading to heterometallic 3d complexes. Overall, substitution at the phosphorus atoms provides a simple strategy to improve the structural adaptability and synthetic versatility of the metallascorpionate framework.



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Modular metalloligands for Cooperative Heterometallic Chemistry

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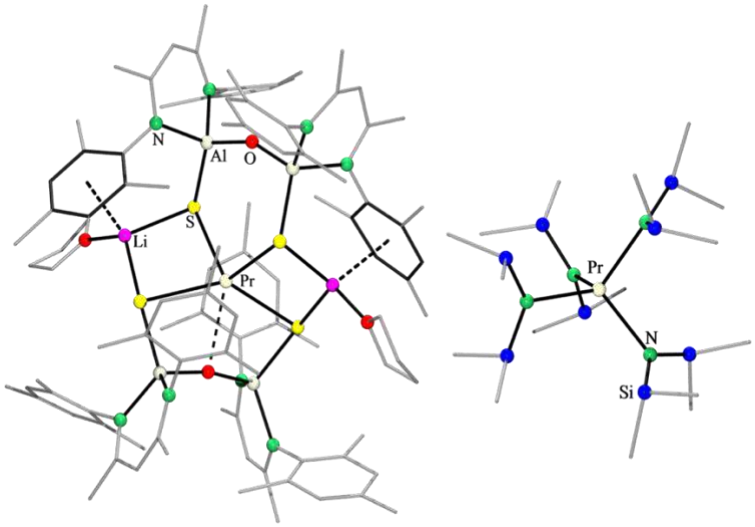
Heterometallic architectures that allow cooperative reactivity remains a central challenge in coordination chemistry [1]. In this work, we present aluminum-centered metalloligands as modular platforms for the assembly of heterometallic frameworks featuring aluminum and selective example of 3d and 4f-block metals. A family of alumoxane-sulfide metalloligands was used to assemble a series of Al–S–M systems, in which the aluminum framework acts as a structurally robust scaffold. Structural studies by single-crystal X-ray diffraction reveal that these metalloligands support unusual coordination motifs, including transannular metal–oxygen interactions and highly organized inorganic cores that enforce proximity between metal centers. Spectroscopic and computational analyses indicate that the aluminum-based scaffold modulates the electronic environment of the coordinated metal, facilitating accessible redox processes and promoting interactions with small molecules.



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TETRAISOPROPYLIMIDODIPHOSPHINATE: ONE SIMPLE PNP-TYPE LIGAND, MUCH OVERLOOKED CHEMISTRY

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Yttrium(III) and zirconium(IV) acetylacetonate precursors have been used in plasma-enhaced chemical vapor depositon (PE-CVD) to produce yttria-stabilized zirconia (YSZ) coatings with enhaced thermal, chemical, and radication resistance. Stabilization of the cubic phase is particularly attractive for thermal barrier coatings and nuclear applications. However, carbon-containing precursors can lead to significant carbon incorporation in deposited films, making precursor decomposition and carbon removal critical for obtaing high-purity YSZ [1].

In this work, we report the synthesis and characterization of Y(III) and Zr(IV) complexes suported by anionic PNP-ligand ($[\{^{i}Pr_2P(O)\}_2N]^-$), as potential alternative precursors for YSZ deposition, with the aim of minimizing carbon incorporation. The synthesis of the proligand, $\{^{i}Pr_2P(O)\}_2NH\bullet H_2O$ (**1**), was optimized through a stepwise route. Interestingly, it crystallized as a monohydrate, a feature not previously reported despite the established synthetic routes [2-4]. The corresponding sodium salt (**2**), and anhydrous Zn(II) (**3**), Y(III) (**4**), and Zr(IV) (**5**) complexes were synthethized and characterized by elemental analysis, multinuclear NMR, FTIR spectroscopy, mass spectrometry, and thermogravimetric analysis (TGA). Complexes **4** and **5** were structurally characterized by single-crystal X-ray diffraction (SCXRD). The $^{31}P\{^{1}H\}$- NMR spectrum of the Zn(II) complex, $[Zn(\{^{i}Pr_2P(O)\}_2N)_2]$, (**3**), exhibited a singlet signal, whereas the Y(III) complex, $[Y(\{^{i}Pr_2P(O)\}_2N)_3]$ (**4**), showed P–Y coupling and adopted a distorted octahedral geometry. Meanwhile, a di-μ-peroxo-bridged dimer $[(\{^{i}Pr_2P(O)\}_2N)_2Zr(O_2)_2Zr(\{^{i}Pr_2P(O)\}_2N)_2]$ (**5**) was isolated, instead $[Zr(\{^{i}Pr_2P(O)\}_2N)_4]$. The IR spectrum showed a band at 801 cm^{-1}, tentatively assigned to ν(O–O), while its $^{31}P\{1H\}$-NMR spectrum displayed two doublets, consistent with inequivalent P environmentes and P–P coupling. Its molecular structure was confirmed by SCXRD. The thermal behaviour of complexes **4** and **5** supported their further evaluation as potential single source precursors (SSPs) for Y_2O_3, ZrO_2 and YSZ deposition. Their performace in YSZ deposition and their ability to minimized carbon incorporation will be explored in future studies.

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Group 3 and 13 Metal Complexes Supported by Phosphasalen and Phosphasalan Ligands: Synthesis, Characterization and Reaction Chemistry.

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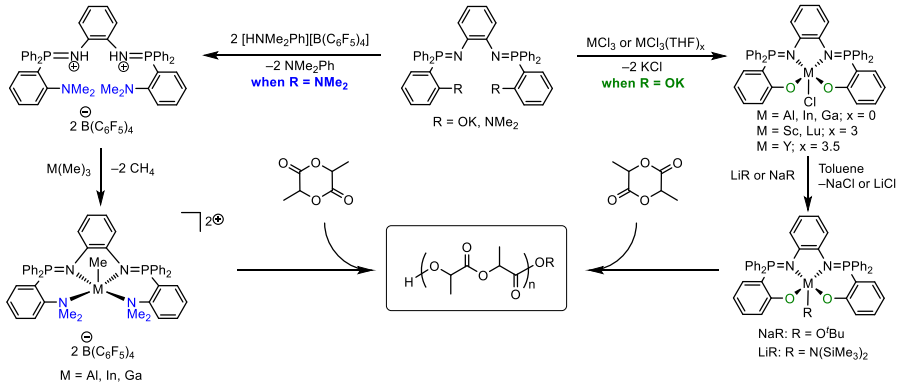
Petroleum-based plastics are ubiquitous in our daily lives; however, they remain in the environment for centuries [1]. Polylactide (PLA) possesses many properites similar to polyolefins, but it is synthesized from renewable sources (*e.g.* wheat, corn, sugar beets) and is biodegradable. PLA is produced from lactide, and exists in three stereoisomers L-LA, D-LA and *meso*-LA. However, it is difficult to produce industrially due to substantial cost to manifacture and the formation of racemic mixtures, causing a loss of crystallinity and low melting point temperature, important properties in polymer synthesis [2]. Phosphasalen ligands contain an iminophosphorane ($RN=PR_3$) functionality, which is robust and strongly electron donating, thereby bind tightly to an array of metals [3]. The Hayes group has reported a route to generate a variety of phosphasalen ligands using a modified Staudinger reaction [4]. This presentation will describe the development of a phosphasalen ligand (**L1** = 1,2-N=PPh_2(2-O-C_6H_4)$_2C_6H_4$) that features a rigid aromatic core. Fine-tuning of steric and electronic properties has increased our understanding of the structure-activity relationship, particularly the role that Lewis acidity plays with respect to reactivity in these systems. Accordingly, the synthesis of a neutral phosphasalan ligand has been targeted (**L2** = 1,2-N=PPh_2(2-NMe_2-C_6H_4)$_2C_6H_4$), which will be used to develop a family of neutral, cationic and dicationic catalysts for ROP of lactide. [5]. The synthesis and characterization of this family of complexes, as well as their reaction chemistry, will be discussed in detail.



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PHOTOINDUCED [2+2] CYCLOADDITION OF A METAL-ORGANIC CAGE INTO AN AMORPHOUS MOF FOR DYE CAPTURE IN WATER

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Metal-organic cages (MOCs) are discrete supramolecular architectures formed through the self-assembly of organic ligands with metal ions, whereas metal-organic frameworks (MOFs) are constructed from similar components but extend into infinite networks[1]. Both classes of materials possess intrinsic cavities or pores capable of selectively recognizing and capturing chemical species[2,3].

In this work, a Pd(II)-based metal-organic cage (MOC) was designed and synthesized from a tricationic ligand, yielding a pseudocubic MOC with an overall +36 charge (PF_6^- as counterions). While photoinduced transformations of metal-organic materials remain relatively unexplored[4], here we report the photoinduced [2+2] cycloaddition reaction of our MOC to obtain a more complex and interconnected polymeric architecture, referred to as “amorphous-Metal-Organic Framework” (aMOF). Although the resulting material is amorphous, it is inferred that MOC cavities are preserved in the polymeric array. Combined with their high positive charges, hydrolyic stability, and water insolubility, both materials exhibit efficient adsorption and separation of dyes from water (also considered as organic pollutants), specifically fluorescein disodium salt (NaFl). Notably, the aMOF exhibits significantly enhanced adsorption kinetics compared with the molecular MOC. Within only 2 minutes, the aMOF reduced the concentration of a 20 ppm (environmentally relevant) aqueous NaFl solution to 3.5% of its initial value, whereas the MOC reduced it only to 53.2% under identical conditions. In addition, the aMOF displayed a higher adsorption capacity (ca. 252.3 mg/g) than the MOC (ca. 195.1 mg/g), highlighting the beneficial effect of the photoinduced transformation on dye uptake performance. Desorption studies were conducted on the NaFl@MOC and NaFl@aMOF systems using methanol as the extraction solvent. The addition of 72 equivalents of NH_4PF_6 resulted in the highest dye release for both materials: 4.89 mg/g and 8.01 mg/g for the MOC and aMOF, respectively. The combined adsorption and desorption performance of these materials demonstrates their potential as reusable adsorbents for aqueous dye remediation and warrants further investigation with a broader range of dye pollutants.

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Session 6. Organometallic Compounds and Catalysis

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C-SCORPIONATE COMPLEXES: FROM COORDINATION VERSATILITY TO SUSTAINABLE CATALYSIS

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Keywords: C-scorpionate, metal complex, catalysis, C-H activation, CO_2 fixation, biomass valorization

Coordination chemistry plays a crucial role in various scientific and industrial fields as it provides insights into the bonding behavior of metal complexes, enabling the design of new materials, catalysts, and fine chemicals with tailored properties and enhanced functionalities.

One class of compounds that has attracted significant attention in recent years is C-scorpionates. These unique ligands, $YX_nC(Rpz)_{3-n}$ (pz = 1*H*-pyrazol-1-yl, n = 0 or 1), with up to three pyrazolyl rings attached to a central carbon atom (Figure 1a), exhibit a scorpion-like structure in the presence of a metal center (Figure 1b,c). Therefore, they exhibit an extraordinary coordination versatility, leading to a wide range of coordination modes and to the formation of metal complexes with distinct geometries, properties, and reactivity.

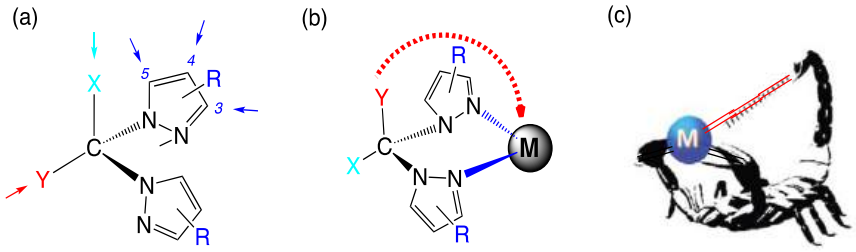

Figure 1. (a) Schematic structure of a C-scorpionate poly(1H-pyrazol-1-yl)methane, $YX_nC(Rpz)_{3-n}$ (pz = 1*H*-pyrazol-1-yl, n = 0 or 1). (b) Coordination modes of $YX_nC(Rpz)_{3-n}$ to a metal (M) centre. (c) Pictorial comparison with a scorpion and its attack on a prey.

C-scorpionate complexes have unlocked an exciting array of applications, namely in challenging reactions of industrial significance. Herein the successful catalytic strategies for using inert carbon dioxide or alkanes as carbon feedstock for the syntheses of functionalized added-value organic compounds, as well as for biomass valorization, are addressed.

Unconventional systems and conditions of sustainable significance, including the use of mechanochemistry and of microwave irradiation are highlighted, and the preferable requirements for a prospective homogeneous or supported catalyst in the above transformations are identified.

Acknowledgements

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PHOTOCATALYTIC DEGRADATION OF PARACETAMOL USING IRON-BASED CATALYSTS SUPPORTED ON SBA-15

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The presence of pharmaceutical residues in aquatic environments is an emerging environmental concern due to their continuous release and occurrence in water and wastewater [1]. Advanced oxidation processes (AOPs) are promising alternatives for the removal of persistent organic contaminants because they generate highly reactive species capable of oxidizing organic molecules [2].

In this work, iron-based catalysts supported on SBA-15 were synthesized with nominal iron oxide loadings of 2, 5, and 10 wt% (2FeSBA-15, 5FeSBA-15, and 10FeSBA-15). The catalysts were characterized by atomic absorption spectroscopy, Fourier-transform infrared spectroscopy (FTIR), porous solid analysis, and diffuse reflectance spectroscopy. Their performance for paracetamol degradation in aqueous solution was evaluated under ultraviolet (UV) irradiation using photolysis, heterogeneous photocatalysis, and heterogeneous photo-Fenton processes. The degradation kinetics were analyzed using a pseudo-first-order model.

The kinetic results showed that the addition of H_2O_2 significantly enhanced paracetamol degradation for all iron-containing catalysts. The highest apparent reaction rate constant was obtained for 5FeSBA-15 + H_2O_2 (0.0757 min^{-1}), followed by 10FeSBA-15 + H_2O_2 (0.0451 min^{-1}) and 2FeSBA-15 + H_2O_2 (0.0340 min^{-1}). In comparison, the rate constants for 2FeSBA-15, 5FeSBA-15, and 10FeSBA-15 without H_2O_2 were 0.0126, 0.0151, and 0.0137 min^{-1}, respectively. The photolysis, SBA-15, and H_2O_2 systems exhibited lower apparent rate constants of 0.0014, 0.0080, and 0.0046 min^{-1}, respectively. The 5FeSBA-15 + H_2O_2 system achieved approximately 98% paracetamol degradation after 60 min of UV irradiation. The enhanced activity is attributed to the generation of reactive oxidizing species, particularly hydroxyl radicals (•OH), through the photo-Fenton reaction. These results demonstrate the potential of 5FeSBA-15 as an efficient heterogeneous photo-Fenton catalyst for paracetamol degradation in aqueous systems.

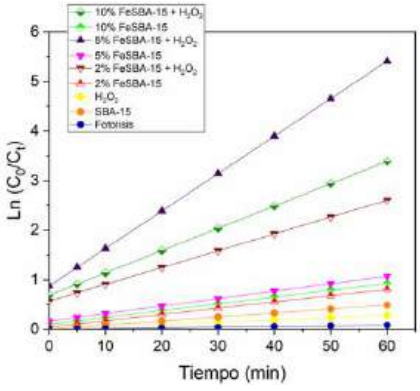

Figure 1. Pseudo-first-order kinetic plots for paracetamol degradation under the evaluated systems.

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FROM MOLECULAR TO HETEROGENOUS CATALYSTS FOR ARTIFICIAL PHOTOSYNTHESIS BY DESIGN

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Julio Lloret Fillol[1,2*]

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Inspired by natural photosynthesis, there is the vision to produce fuels and chemicals using Earth's abundant molecules (such as H_2O, CO_2, N_2) and renewable energy.[1] Understanding these processes is crucial for developing efficient small molecule transformations.[2] In this context, we will discuss our efforts to develop well-defined coordination complexes that act as efficient homogeneous catalysts for CO_2 reduction, activation of alkyl chlorides and other transformations identified during the process.[3] These transformations share that are mediated by low valent metal complexes.[4-5]

For CO_2 reduction, I will present highly active manganese-based catalysts that operate effectively at very low CO_2 concentrations and demonstrate how the selectivity of CO_2 reduction can be tuned from CO to HCO_2H. The development of stable and selective catalysts for CO2 reduction has needed a deep insight of the CO_2 reduction mechanisms by metal complexes, which has been instrumental in designing more efficient catalysts and find reaction conditions to shift the selectivity to yield formate. We will also discuss how scale-up systems in the context of the EU project PHOTOSINT.

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FROM MOLECULAR TO POLYMERSOME-BASED SYSTEMS FOR PHOTOCATALYTIC CO_2 REDUCTION

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Carla Casadevall,[1,2*], Laura Velasco-Garcia[1,2], Edelman J. Espinoza-Suárez[1,2], Akhmet Bekaliyev,[1,2], Leonardo Quesada-Román[1,2]

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The sustainable synthesis of fuels and chemicals using sunlight as driving force and readily available feedstock such as H_2O and waste CO_2 provides a potential pathway to mitigate increasing CO_2 emissions and transitioning toward a greener chemical industry. In this context, natural photosynthesis is a source of inspiration and has led to the evolving and multidisciplinary field of artificial photosynthesis (AP).[1-4] However, when designing bioinspired photocatalytic platforms for AP, nature's compartmentalization is sometimes overlooked. We are studying how this key structural feature can be translated to develop bioinspired AP systems.[4] We are developing polymersomes functionalized with (photo)catalysts to produce solar fuels and chemicals in aqueous media using solar energy as driving force.[5] We have developed a novel family of asymmetric porphyrin and phthalocyanine complexes bearing Co, Ni, and Fe 1st row transition metals for photocatalytic CO_2 reduction (CO_2R) in combination with Ir- and Cu-based photosensitizers and organic dyes, under visible light irradiation in organic mixtures in presence of a sacrificial electron donor.[5] The phthalocyanine complexes show a remarkable photocatalytic activity and selectivity for photocatalytic CO_2R to CO in homogeneous conditions, even with 10% of water. In contrast, the porphyrin complexes show remarkable activity and selectivity for methane production. Moreover, to further explore the applicability and increase the stability of these systems, we have anchored both the CO_2R catalyst and photosensitizer onto the membrane of polymersomes, developing the first polymersome for compartmentalized photocatalytic CO_2R.[5] The effect of anchoring and the nature of the photosensitizer allows to tune the selectivity of the photocatalytic reaction to obtain only CO_2R derived products in water, suppressing the normally competing H_2 evolution reaction. Mechanistic studies are ongoing to rationalize these differences in reactivity between homogeneous and heterogenized systems.

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PHOTOCATALYTIC DEGRADATION OF PARACETAMOL USING IRON-BASED CATALYSTS SUPPORTED ON SBA-15

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The presence of pharmaceutical residues in aquatic environments has become an emerging environmental concern due to their continuous release and widespread occurrence throughout the urban water cycle [1,3]. Some pharmaceutical compounds have also been detected in drinking water, highlighting the need for effective treatment technologies for their removal [1,4]. Advanced oxidation processes are promising alternatives for the degradation of persistent organic contaminants because they involve the generation of highly reactive species capable of oxidizing organic molecules [2].

The objective of this work was to synthesize and evaluate solid iron-based catalysts supported on SBA-15, with nominal iron oxide loadings of 2, 5, and 10 wt% (2FeSBA15, 5FeSBA15, and 10FeSBA15), for the degradation of paracetamol in aqueous solution by photolysis, heterogeneous photocatalysis, and heterogeneous photo-Fenton processes under ultraviolet irradiation. The synthesized catalysts were characterized by atomic absorption spectroscopy, Fourier-transform infrared spectroscopy (FTIR), porous solid analysis, and diffuse reflectance spectroscopy. Their catalytic activity was evaluated by monitoring the degradation of paracetamol, and the experimental data were fitted to a pseudo-first-order kinetic model to determine the apparent reaction rate constants.

Among the evaluated systems, 5FeSBA15 in the presence of H_2O_2 exhibited the highest catalytic activity, with an apparent pseudo-first-order rate constant of 0.0757 min^{-1}, achieving approximately 98% paracetamol degradation after 60 min of UV irradiation. The enhanced degradation performance in the presence of H_2O_2 is attributed to the generation of reactive oxidizing species, particularly hydroxyl radicals (•OH), which promote the oxidation and transformation of paracetamol. For comparison, the rate constants obtained for 2FeSBA15 + H_2O_2 and 10FeSBA15 + H_2O_2 were 0.0340 and 0.0451 min^{-1}, respectively. These results demonstrate the potential of the 5FeSBA15 catalyst for the degradation of paracetamol in aqueous systems through heterogeneous photo-Fenton processes.

From Electronic Structure to Photochemical Function: Molecular Design of Re(I) and Mn(I) Tricarbonyl Complexes

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Transition-metal carbonyl complexes offer versatile platforms for controlling light-driven molecular processes through the modulation of their coordination sphere and ligand framework, **Figure 1** [1]. This work explores *fac*-$[M(N\hat{}N)(CO)_3L]^{0/+}$ complexes (M = Re(I), Mn(I)) to establish relationships between molecular structure, electronic properties, biological and photochemical reactivity. Particular emphasis is placed on N^N-chelating ligands capable of modulating the electronic structure of the metal center and on functional architectures displaying spectroscopic sensing, photoinduced processes [2, 3], and charge-transfer excited states. Spectroscopic, time-resolved and computational approaches provide insight into metal-ligand interactions and the factors governing excited-state behavior [4]. These concepts are extended to Mn(I) tricarbonyl systems designed as visible-light-responsive photoCORMs and multifunctional photoactive platforms. The integration of CO release with photosensitized singlet oxygen generation illustrates how ligand and metal-center design can be used to couple distinct photochemical pathways within a single molecular framework, with potential applications in sensing and light-activated therapy.

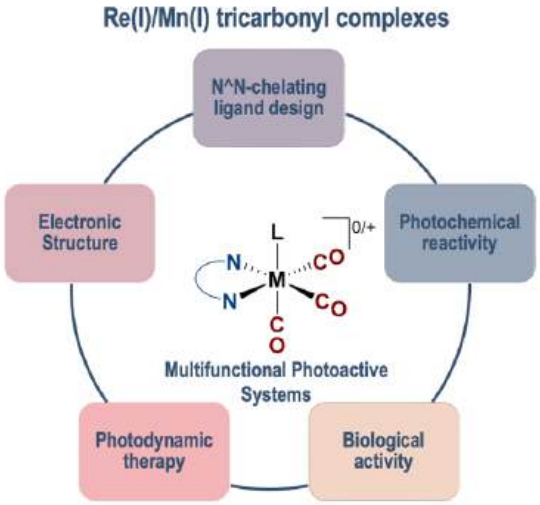

Figure 1. General structure of Re(I)/Mn(I) tricarbonyl complexes

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Synthesis and application of Cu(I) complexes featuring NN-type bidentate ligands in CO_2 electroreduction.

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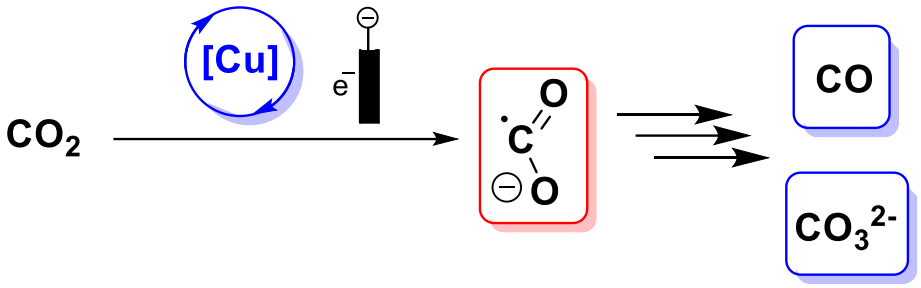
Abstract. The use of carbon as the primary resource for generating various energy sources and powering daily activities increases anthropogenic greenhouse gas emissions, predominantly CO_2 (currently at a concentration of 431.44 ppm) [1], which are the main drivers of global issues such as climate change and planetary temperature rise. CO_2 is a highly stable and chemically inert molecule due to the nature of its chemical bonds and its linear geometric structure, making its activation a significant challenge. To address this, the synthesis of novel, cost-effective, and selective catalysts is sought for processes such as the electrochemical CO_2 reduction reaction (CO_2RR), where lowering the overpotential—compared to conventional bare electrodes—is required to improve the process. This work reports the synthesis and characterization of several Cu(I) complexes featuring NN-type bidentate auxiliary ligands. These complexes were evaluated as catalytic precursors in the CO_2RR. The electrochemical systems exhibit a decrease in the activation potential for the CO_2 molecule, alongside key experiments confirming the formation of the CO_2 radical anion (CO_2•−), which align with previous reports regarding its reactivity.[2]



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Functionalized Mesoionic Carbenes: Versatile Ligands for Transition Metals and Homogeneous Catalysis

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The use of mesoionic carbenes (MICs) in transition metal chemistry has experienced an exponential growth over the last two decades [1]. Because of the accessible modification of their structural features, a vast amount of metal complexes with MICs have been reported and numerous applications found in catalysis and other related areas. Owing to the commonly practiced routes, most of the MIC derived complexes based on the imidazole or 1,2,3-triazole frameworks feature alkyl or aryl groups as substituents [2]. For several years our group has been actively searching for platforms featuring diverse substitution patterns in order to tune their electronic and steric properties [3]. Furthermore, we have been actively designing carbene platforms capable of holding two different metal centers within the same ligand [4]. Our interest in these particular systems arises from the documented demonstration on how the use of two different metal complexes can provide a better catalyst system than the constituent monometallic units. One approach to enable the selective insertion of two (or more) metal centers relies on the design of ligands with at least two distinct sites to sequentially coordinate the metal ions. This can be assessed by exploiting the preference of certain metal centers for specific coordinating sites according to the concept of soft and hard donors. Another possibility involves the design of a mixed framework in which a masked (or protected) functionality permits the selective inclusion of a first metal before the release of the free version of the ligand for coordination of the second metallic ion. In this regard, the use of azolium salts (precursors for MIC ligands) bearing additional sigma-donor functionalities offers an excellent alternative for the stepwise construction of heterobimetallic species. We present in this work, the design and construction of a series of highly functionalized MIC ligands and the application of their resulting mono- and heterometallic species in homogeneous catalysis. The structural diversity in solution and solid state of all new complexes will be discussed in detail.

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SELECTIVITY CONTROL IN Pd-CATALYZED ISOPRENE TELOMERIZATION

Jordi Colavida,[1,2] Ricardo G. Penido,[3] Ana Collado,[2] Josep M. Ricart,[4] Cyril Godard,[4] Carmen Claver,[1,4] Jorge J. Carbó,[4] Eduardo N. dos Santos,[3] Sergio Castillon[1,5]

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The telomerization of dienes is a transition metal catalyzed multicomponent reaction that consists in the reaction of two molecules of a diene with the subsequent addition of a nucleophile, such as an alcohol, an amine, an acid, or water, to form highly valuable intermediates [1]. Butadiene is the simplest and widely studied diene, and butadiene telomerization is today an industrial process key for 1-octene production [2], and several companies have plants for this process. Butadiene telomerization can afford three different products, linear, branched and elimination, with the linear telomer presenting the most interesting properties. However, for isoprene (2-methylbutadiene), the simplest example of non-symmetric diene, the telomerization process can yield up to 12 isomers, making this process a formidable challenge. In this case linear telomers are preferably obtained, and are also the more appreciated, since the C-10 products obtained are structurally related to monoterpenes that are key products in the flavors and fragrances industry. In this communication we will discuss the factors controlling the regioselectivity, which allowed to obtain selectively up to 3 isomers [3]. A comparison with related results obtained using nickel as catalyst will be also presented.

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Z-Selective Cu-NPs Catalyzed Alkyne Direct Semihydrogenation

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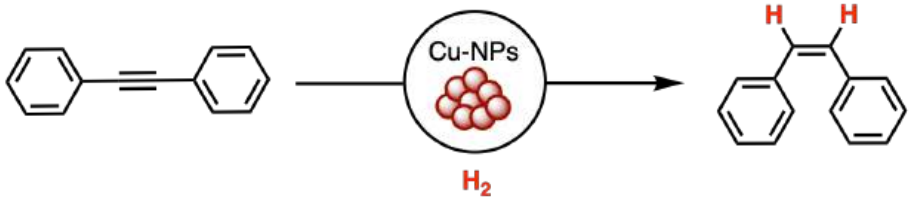
Over the past few years, nanoparticles have emerged as versatile tools used for the strategic design of advanced nanomaterials and molecular building blocks [1,2]. Among these applications, the catalytic stereoselective semihydrogenation of alkynes to *Z*-alkenes is an efficient strategy for obtaining critical intermediates in organic synthesis and biologically active target compounds [3-5]. Herein, we report the development of *in situ* generated copper nanoparticles for the highly efficient semihydrogenation of internal alkynes. This reaction proceeds in the presence of catalytic amounts of [Cu(dippe)(PPh_3)(k^1-NO_3)], $PhSiH_3$, and AcOK in THF under mild conditions, using molecular hydrogen. This protocol provides access to *Z*-alkenes with high stereoselectivity and completely suppresses side reactions such as overreduction or hydrosilylation. The broad applicability and functional-group tolerance of the catalytic system were tested across a diverse substrate scope, including functionalized internal alkynes, terminal alkynes, and dialkynes.



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Iron-promoted synthesis of novel fluorescent *5H*-Thiazolo[3,2-*a*]pyridin-5-ones

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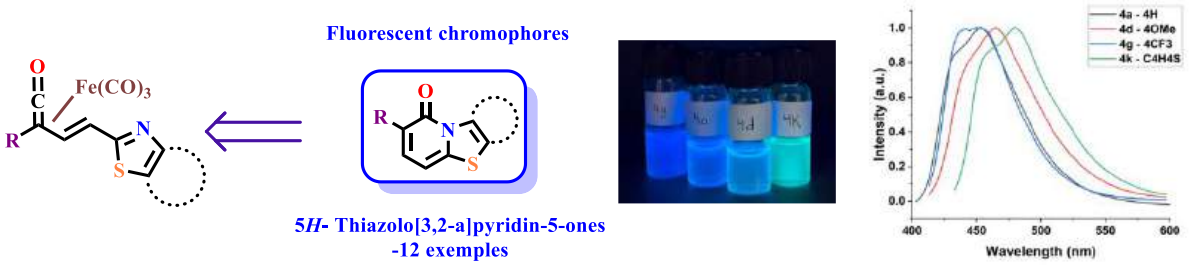
5H-Thiazolo[3,2-a]pyridin-5-ones are heterocyclic systems of considerable interest in biomedical research owing to their pharmacological and photophysical properties,[1] which have enabled their potential applications as biological probes,[2] sensors for biogenic molecules[3] and white-light-emitting diodes.[4] Here, we present a new synthetic approach for obtaining a variety of this target heterocyclic compounds based on the use of (η^4-vinylketene)-$Fe(CO)_3$ complexes as key intermediates. This methodology is general and tolerate the incorporation of different aryl and heteroaryl fragments and enabled the synthesis of a library of 12 new fluorophores. Systematic variation of electron-donating and electron-withdrawing substituents allowed modulation of the emission color, while the resulting compounds exhibited large Stokes shifts and high quantum yields. Overall, these results establish a clear relationship between the electronic nature of the substituents and the emission properties of this new family of fluorophores. These findings provide a rational basis for the design of fluorophores with tunable and predictable photophysical properties and contribute to the development of new molecular platforms with potential applications in optical and optoelectronic materials.[5]



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Synthesis and Application of Co(I) Complexes in the Catalytic Hydrogenation of Levulinic Acid and Furfural.

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Biomass-derived levulinic acid (LA) and furfural (FF) are promising alternatives to traditional fossil-fuel-based raw materials for applications such as biofuels. In this work, we present the synthesis and characterization of highly reactive compounds in biomass valorization. Co(I) complexes of the type [(diphosphine)CoPPh$_3$Cl], which are synthesized using commercially available low-cost precursors and feature bidentate ligands with different bite angles and electronic and steric parameters.

The Co(I) complexes were applied in the direct hydrogenation of LA and FF to produce selectively γ-valerolactone (GVL) and tetrahydrofurfuryl alcohol (THFA), respectively, using relatively mild reaction conditions, a non-noble metal system and through the in-situ formation of cobalt nanoparticles, which allows a high dispersion and TOF´s of 41.7 for both system at its respective optimal conditions [1].

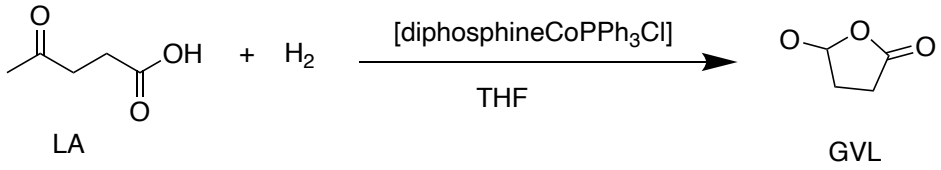

Figure 1. Selected example of the conversion of LA to GVL. 120 º and H_2 300 psi, 99 % yield.

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PHOTOCHEMICAL MEANS OPEN UP NEW PATHWAYS FOR NICKEL CATALYSIS

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The Bahamonde group is interested in the development and mechanistic understanding of Ni-catalyzed processes that involve light-mediated steps—either to generate radicals that can be trapped enantioselectively or to promote C–heteroatom reductive eliminations at room temperature. Like other first-row transition metals, Ni participates in both one- and two-electron processes, resulting in broad and distinct reactivity while complicating our mechanistic understanding. To address this challenge, our research prioritizes gaining mechanistic insight as a foundation for rational catalyst and reaction design.

Synthesis of Copper(II) Complexes with Schiff Base Ligands Derived from Amino Acids and Their Evaluation as Catalysts in the Cyclopropanation of Styrene

Luis-Angel Barreras-Contreras[1], Karla-Alejandra Lopez-Gastelum[2], Rocío Sugich-Miranda[3], Alejandra-María Durazo-Garcia[1], Felipe Medrano-Valenzuela[3], Enrique-Fernando Velazquez-Contreras[1], Fernando Rocha-Alonzo[3]

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Asymmetric catalysis is of significant importance in chemistry due to the relevance of stereospecificity in molecular design, particularly in the pharmaceutical, agrochemical, and materials industries [1]. Chiral cyclopropanes are valuable structural motifs with diverse applications, including their use in enzyme inhibitors, antibiotics, antiviral and antitumor agents, and neuroactive compounds. One of the most important approaches for the synthesis of chiral cyclopropanes is the transition-metal-catalyzed cyclopropanation of olefins using diazo compounds [2].

In this project, new copper(II) complexes were synthesized using chiral ligands derived from reduced Schiff bases obtained from the amino acids L-phenylalanine, L-alanine, L-tryptophan, L-leucine, and L-isoleucine [3]. The ligands were purified by precipitation and liquid–liquid extraction, with their purity monitored by thin-layer chromatography (TLC), and characterized using infrared (IR), UV–Vis, and ^{1}H NMR spectroscopy, mass spectrometry, and melting point determination. The resulting copper(II) complexes were evaluated as catalysts for the cyclopropanation of styrene using a diazo precursor. The complexes exhibited catalytic activity, affording the corresponding cyclopropane product in good yields.

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Copper(I) Diphosphine Cyanide Compounds: Nuclearity and Photocatalytic Activity

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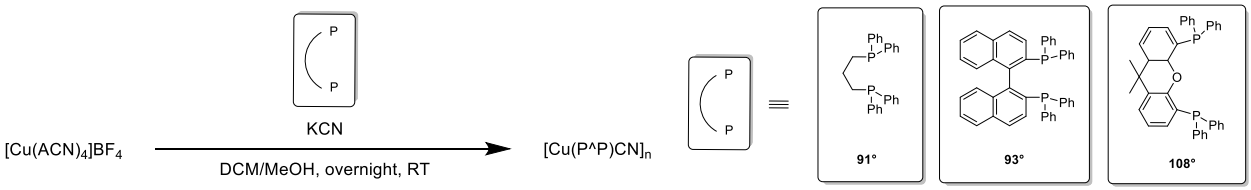
The development of photocatalysts based on Earth-abundant metals is a key objective in advancing sustainable catalysis.[1] Among these, Cu(I) diphosphine complexes have emerged as attractive alternatives to noble-metal photosensitizers owing to the low cost, high natural abundance, and versatile coordination chemistry of copper, together with the extensive library of available diphosphine ligands.[2] Despite their widespread application, many catalytic systems rely on the *in situ* generation of the active Cu(I) species, leaving the identity of the actual coordination environment and nuclearity of the photocatalyst poorly defined. This issue is particularly relevant for cyanide-containing Cu(I) complexes, where the bridging ability of the cyanide ligand gives rise to a range of structural motifs, including one-dimensional coordination polymers for dppb derivatives,[3] and discrete trinuclear species for dppp analogues.[4] This contribution presents the synthesis, characterization, and photoactivity investigation of a family of Cu(I) cyanide complexes of general formula $[Cu(P\hat{}P)CN]_n$ (P^P = Xantphos, dppp, BINAP). The relationship between diphosphine ligand architecture, complex nuclearity, and the resulting electronic and excited-state properties will be discussed. Preliminary studies on the application of these well-defined complexes as photo- and electrocatalysts for visible-light-driven transformations will also be presented.



Scheme 1. Synthesis of title complexes.

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New Mechanistic Insights into NHC-Catalyzed Glycerol Transesterification

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In recent years, research on producing value-added compounds from biomass-derived waste has become a major field of study. Glycerol valorization is part of this effort, as glycerol is the main byproduct of biodiesel production. Transesterification with dimethyl carbonate (DMC) to produce glycerol carbonate is one of the most promising routes.[1] Both homogeneous and heterogeneous catalysts have been used to promote this reaction. Among them, N-heterocyclic carbenes (NHCs) stand out as organic molecules used as organocatalysts due to their amphiphilic and stereoelectronic properties.[2] Despite the interest in these compounds, few studies have thoroughly investigated their reaction pathway.[3] Therefore, this work presents an experimental and computational mechanistic study of the NHC-organocatalyzed transesterification of glycerol with DMC using free IMes as a model catalyst.

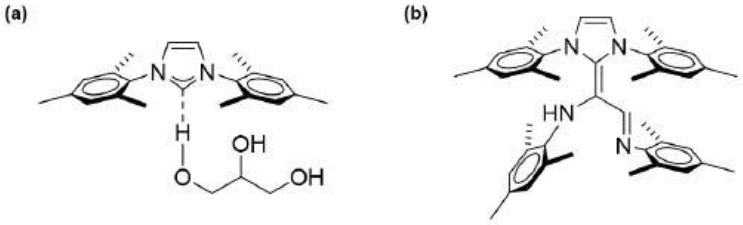

Figure 1. (a) Adduct formed between free IMes and glycerol. **(b)** IMes aza-Breslow-like compound.

The results revealed the formation of an IMes–glycerol adduct (Figure 1a) as the first intermediate in the reaction mechanism, which was characterized by NMR (^{1}H NMR, ^{13}C NMR, HSQC, HMBC, and NOESY). DFT calculations not only corroborated its formation (4.0 kcal mol^{-1}) but also showed that a Breslow-type intermediate between the carbene and DMC is energetically unfavorable at room temperature (59.2 kcal mol^{-1}). These results support a new mechanistic proposal in which alcohol activation occurs as the first step and will be discussed in the presentation.[4] More remarkably, experimental investigation of the mechanism enabled the synthesis and isolation of an IMes-derived aza-Breslow-like compound (Figure 1b),[5] which, to the best of our knowledge, has not been previously reported. The new compound was characterized by single-crystal XRD, NMR, and HRMS.

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UNUSUAL REGIOSELECTIVITY IN STYRENE HYDROFORMYLATION CATALYTIC SYSTEMS FOR LINEAR ALDEHYDE PRODUCTION

Carmen Claver[1,2], Benedetta Palucci [2], Aitor Gual[2], Gonzalo D. Nuñez [1] Mario Villares,[1] Maria Besora,[1] Jorge J. Carbó,[1] Cyril Godard [1]

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The production of aldehydes from olefins via hydroformylation is one of the most important industrial processes using homogeneous catalysis. Rh catalysts modified with phosphorus ligands allow to control the regioselectivity and stereoselectivity in the hydroformylation reaction to obtain the desired aldehydes [1]. Styrene is often applied as model substrate for the hydroformylation of vinyl arenes because of the formation of branched aldehyde containing a stereogenic center which offers a synthetic route to anti-inflammatory drugs. In the last years, however, the interest of the linear aldehydes derived from styrene to obtain intermediates in pharmaceuticals and fragrances has increased. It has been shown that ligand modifications lead to the linear aldehyde as the majority product [1-3].

Despite the efficiency of syngas based hydroformylation processes, an alternative “syngas surrogates” emerged as a compelling strategy using reagents which can act as “in situ” sources of CO/H2 avoiding the problems of syngas directly handling [1,4]. In this presentation the optimization of a Pd system using formaldehyde syngas surrogate for styrene hydroformylation is described. Linear aldehydes can be obtained in up to 97% conversion, and l/b ratio >99. Reaction monitoring shows hydrogenation in competence with hydroformylation. Computational studies allow us to propose a new catalytic cycle.

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Divergent Reactivity of Ru and Os Pincer Complexes in the Chemoselective Reduction of Unsaturated Carbonyl Compounds

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The chemoselective hydrogenation of multifunctional substrates provides a valuable platform for probing the reactivity of transition-metal catalysts. In this context, pincer complexes offer a well-defined environment in which the nature of the metal center and reaction conditions can strongly influence catalytic selectivity. Herein, we investigate the reactivity of selected Ru and Os pincer complexes (Gusev's catalysts) in the selective reduction of unsaturated esters and aldehydes, focusing on the competing hydrogenation of carbonyl and olefin functionalities.

A series of catalytic reactions was performed using methyl 10-undecenoate, myrtenal, and cinnamaldehyde as representative substrates. Both hydrogenation [1] and transfer hydrogenation [2] were explored, the latter employing ethanol as a hydrogen donor. The catalytic results revealed pronounced differences between the ruthenium and osmium systems. In particular, selected Os pincer complexes exhibited remarkable chemoselectivity in transfer hydrogenation, promoting efficient carbonyl reduction while leaving the C–C double bond largely unaffected. The comparison of selectivity among the Ru and Os provides new insight into the reactivity of this class of organometallic systems.

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Effect of Keggin Lacunarity on Polyoxometalate-Based Catalysts Supported on Methylimidazolium-Functionalized Mesoporous Silica for Fused N-Heterocycle Synthesis

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Keggin-type polyoxometalates (POMs) offer versatile platforms for catalyst design owing to their structural and electronic tunability [1,2]. Herein, saturated and mono-, di- and tri-lacunary phosphotungstate Keggin POMs were immobilised on covalently methylimidazolium-functionalised mesoporous silica (MIM-SBA-15) and evaluated for the synthesis of fused N-heterocycles. Phosphotungstic acid (HPW_{12}) and tetrabutylammonium (TBA) salts of the corresponding lacunary POMs were incorporated by impregnation, followed by controlled drying and thermal treatment [3,4]. The resulting materials were characterised by N_2 adsorption–desorption, powder X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS. Catalytic performance was evaluated in the condensation of aldehydes with 2,3-diaminophenazine, affording fused N-heteroaromatic products through sequential condensation, dehydration and cyclisation processes. This approach aims to establish relationships between Keggin lacunarity, POM–support interactions, and catalytic performance in fused N-heterocycle synthesis.

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Pincer palladacycle as efficient catalysts for carbonylative Suzuki cross-coupling using $Fe(CO)_5$ as a CO surrogate

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Pincer-type palladacycles have emerged as versatile catalysts in cross-coupling reactions due to their high thermal stability and tunable electronic properties. In this work, we report the synthesis of a series of pincer palladacycles and their evaluation as catalysts in the Suzuki-carbonylative coupling of aryl iodides with arylboronic acids, using $Fe(CO)_5$ as a safe and convenient CO surrogate.

Pincer-type palladacycles have emerged as versatile catalysts in cross-coupling reactions due to their high thermal stability and tunable electronic properties. This work describes the synthesis of a series of pincer-type palladacycles and their evaluation as catalysts in the carbonylative Suzuki coupling of aryl iodides and arylboronic acids, using $Fe(CO)_5$ as a safe and practical substitute for CO.

Reaction conditions were systematically optimized by varying the time, catalyst loading, base, solvent, CO source, and CO concentration. Under the optimal conditions identified (0.5 mol% catalyst, K_2CO_3 as base, toluene as solvent, 0.4 equivalents of $Fe(CO)_5$, 3 h at 80 °C), the desired diaryl ketones were obtained with excellent yields and selectivities. The catalytic system demonstrated good tolerance toward a wide range of functional groups—including electron-withdrawing and electron-donating substituents—as well as sterically hindered substrates.

The synthetic utility of the methodology was further demonstrated by the preparation of the bioactive compound (4-methoxyphenyl)(3,4,5-trimethoxyphenyl)methanone, a known inhibitor of tubulin polymerization, which was obtained in 42% yield with complete selectivity.

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Unsymmetrical pincer type palladacycles (Pd-CNS) based on ligands arylhydrazones-alkylthioether as carbonylative Sonogashira cross-coupling catalysts

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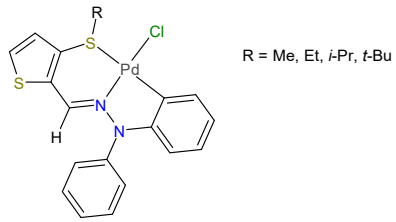
A family of four asymmetric pincer-type palladacycles based on arylhydrazone-thioether ligands was synthesized and fully characterized using conventional spectroscopic techniques (Scheme 1). These palladacycles were employed as catalysts in the carbonylative Sonogashira cross-coupling reaction.



Scheme 1. Structure of synthetized palladacycles.

Following the synthesis of palladacycles, catalytic studies were conducted to evaluate their activity and scope as catalysts in carbonylative Sonogashira coupling reactions.

The catalytic system was optimized using the coupling of 4-iodoanisole, phenylacetylene, and $Mo(CO)_6$ (as a surrogate carbon monoxide source) [1] via an experimental design—specifically, a 2^{5-1} fractional factorial design with a center point—to determine optimal reaction conditions, such as solvent, base type, precatalyst concentration, temperature, and reaction time.

The catalytic system demonstrated excellent performance, successfully activating a wide range of aryl iodides and terminal alkynes with diverse electronic properties, while achieving high conversions and selectivities for carbonylation products (Scheme 2).

Scheme 2. Catalytic system employing palladacycles as precatalysts.

Finally, the efficiency of the catalytic system was compared with other commercial palladium sources under the same conditions; our precatalyst showed similar conversion but significantly better selectivity than the other precatalysts.

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Acknowledgements (10 pt)

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And we thank to M. Sc. Pablo Hernández Matamoros for the realization of some gas chromatography analysis.

One-Pot Catalysis Enabled by a Hybrid Chiral Diene/Phosphine Ligand

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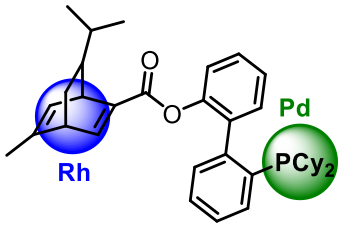
One-pot multicomponent systems have emerged as a powerful strategy to efficiently access intricate structures while reducing the waste, time, and energy associated with the workup and isolation of intermediates.[1,2] The most common approach relies on the use of individual catalysts, while the integration of mechanistically independent catalytic fragments into a single framework remains largely underexplored, with only a few heterobimetallic examples reported to date.[3-5] The design of L1, a hybrid chiral diene/phosphine ligand, enables orthogonal relay catalysis through selective coordination of the chiral diene to rhodium and of an electron-rich biaryl phosphine to palladium, allowing tandem Rh-catalyzed asymmetric arylation (RCAA) and Pd-catalyzed cross-coupling. The chemo- and stereoselective transformation achieved at low catalyst loading and an almost stoichiometric metal/ligand ratio highlights the potential of this approach to access valuable products. Each fragment of L1 provides access to a pool of yet-to-be-explored reactivity, positioning it as a multifunctional framework for new organic synthesis methodologies.



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Acknowledgements
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Reactivity studies of heterobimetallic Fe-Cu complexes supported on dipyrrin and tpa

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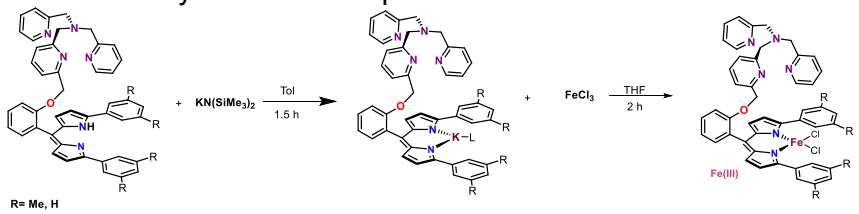
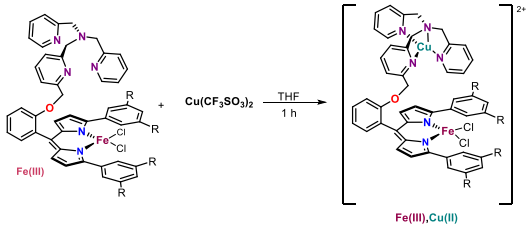
Heterobimetallic Fe-Cu complexes with Fe-porphyrin tethered to a Cu-tpa have been studied by Karlin for their use as cytochrome C oxidase analogues that mimic the activity of the active site (tpa = tris(2-pyridylmethyl)amine).[1] While the majority of work on this kind of Fe-Cu complexes has been focused on the use of porphyrin as the platform for Fe, we have focused on the use of dipyrrin moiety as an open version of the porphyrin to simplify the purification, enhance the yield, and increase the scale.[2] In this work, we will discuss the synthesis of two binucleating ligands and their Fe-Cu complexes, having variations in the aryl group of the dipyrrin fragment (Scheme 1). Studies on electrocatalytic reduction of CO_2 will be included, along with DFT calculations of possible adducts of C_2 products. Additionally, the synthesis of mononuclear Cu(I), Cu(II) and Fe(III) complexes on dipyrrin ligands was developed to compare their activity on electrochemical CO_2 reduction.[3]

Scheme 1. Synthesis of complexes.





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Hydroboration of Benzophenone Mediated by Tripodal Lithium and Group 13 Metal Complexes

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In recent years, the development of catalysts based on earth-abundant and low-toxicity metals has attracted considerable attention as an alternative to traditional transition-metal systems[1,2]. The focus of this project is the homogeneous catalytic hydroboration of benzophenone using complexes containing a Lewis acidic main-group metal (M = Al, Ga, In) in close proximity to lithium through (2-(dimethylamino)phenyl buttresses. These metal complexes represent an attractive platform because their cooperative and highly tunable architectures can promote efficient substrate activation. In this work, we present the synthesis of lithium–triel tris(aminoaryl) complexes linked by (2-(dimethylamino)phenyl groups. The complexes were characterized by IR, by IR, 1H, 13C,and 27Al NMR spectroscopy, as well as single-crystal X-ray diffraction. Structural analysis revealed a tetrahedral geometry around the group 13 metal center and a trigonal planar geometry around the lithium center. The catalytic activity of these complexes was evaluated in the hydroboration of benzophenone, showing quantitative conversion within a short reaction time. These results demonstrate that lithium–triel complexes exhibit promising catalytic activity for hydroboration reactions while employing earth-abundant and low-toxicity metals. The study of these compounds is particularly interesting not only for understanding the role of heterometallic cooperation in catalysis, but also for exploring how the identity of the group 13 metal influences reactivity, selectivity, and catalytic efficiency. Such insights could contribute to the rational design of new main-group catalysts for sustainable reduction chemistry.

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Synthesis of a new Lindqvist-type polyoxomolybdate with a pyridylamine ligand as the counterion

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Polyoxometalates (POMs) are anionic inorganic aggregates primarily composed of oxygen and transition metals in high oxidation states. Within this broad family of metal clusters lies the subgroup of ammonium polyoxomolybdates, consisting of an inorganic polyanion of the form $[Mo_xO_y]^{n-}$ and protonated amines acting as counterions [1]. Generally, these metal clusters can be synthesized by the acidification of oxometallic salts or through solvothermal treatment of pre-synthesized POMs in the presence of organic ligand [2,3]. Hexanuclear clusters $[Mo_6O_{19}]^{2-}$ belong to a family known as Lindqvist-type POMs, which feature a superoctahedral structure composed of six octahedral MO_6 oxometallic subunits. POMs have been employed as catalysts for epoxidation reactions and the sulfoxidation of sulfur-containing compounds, the latter being of particular interest due to its application in the deep desulfurization of fuels [4].

Herein, we present a novel synthesis route to a Lindqvist-type POM promoted by a pyridylamine ligand. This was achieved under neutral pH conditions through the reaction of *N*-benzyl-*N*-(2-methylpyridyl)cyclohexylamine with $MoO_2Cl_2(DMF)_2$ under solvent reflux, yielding the ammonium hexamolybdate $Mo_6O_{19}(C_{19}H_{25}N_2)_2$ (**POM1**). The resulting POM was characterized by conventional spectroscopic techniques, and suitable single crystals were obtained for XRD analysis. The newly synthesized POM exhibited low catalytic activity in the epoxidation reaction of *cis*-cyclooctene, achieving a maximum conversion of 37%. In contrast, it showed moderate catalytic performance in the oxidation of dibenzothiophene (DBT), reaching conversion above 90% after 48 hours.

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Functionalized Mesoionic Carbenes: Versatile Ligands for Transition Metals and Homogeneous Catalysis

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The use of mesoionic carbenes (MICs) in transition metal chemistry has experienced an exponential growth over the last two decades [1]. Because of the accessible modification of their structural features, a vast amount of metal complexes with MICs have been reported and numerous applications found in catalysis and other related areas. Owing to the commonly practiced routes, most of the MIC derived complexes based on the imidazole or 1,2,3-triazole frameworks feature alkyl or aryl groups as substituents [2]. For several years our group has been actively searching for platforms featuring diverse substitution patterns in order to tune their electronic and steric properties [3]. Furthermore, we have been actively designing carbene platforms capable of holding two different metal centers within the same ligand [4]. Our interest in these particular systems arises from the documented demonstration on how the use of two different metal complexes can provide a better catalyst system than the constituent monometallic units. One approach to enable the selective insertion of two (or more) metal centers relies on the design of ligands with at least two distinct sites to sequentially coordinate the metal ions. This can be assessed by exploiting the preference of certain metal centers for specific coordinating sites according to the concept of soft and hard donors. Another possibility involves the design of a mixed framework in which a masked (or protected) functionality permits the selective inclusion of a first metal before the release of the free version of the ligand for coordination of the second metallic ion. In this regard, the use of azolium salts (precursors for MIC ligands) bearing additional sigma-donor functionalities offers an excellent alternative for the stepwise construction of heterobimetallic species. We present in this work, the design and construction of a series of highly functionalized MIC ligands and the application of their resulting mono- and heterometallic species in homogeneous catalysis. The structural diversity in solution and solid state of all new complexes will be discussed in detail.

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Photocatalytic Acceptorless Dehydrogenation of Ethers by Nickel Hydride Complexes

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Alkenes, which serve as a critical platform from which much of the chemical industry is built upon, are generally prepared by high-temperature cracking reactions. Cracking is not compatible with functionalized hydrocarbons, however, with ethers undergoing C–O cleavage instead of dehydrogenation at high temperatures. This limits large-scale access to vinyl ethers and enol ethers that serve as key intermediates to small molecules and polymer materials. Here, we present a unique photocatalytic acceptorless dehydrogenation of ethers that provides a new route to functional alkenes. Linear, cyclic, and polymeric ethers are all viable substrates, including several biomass-derived ethers that could be intermediates in biorefineries. A range of alkenyl ethers were prepared, including several simple molecules that have never been prepared before. Comparisons of catalyst structures show that bis(diphosphine) nickel hydrides with small aliphatic substituents give the highest turnover numbers. Competing bimetallic H_2 evolution were identified as a key side reaction that deactivates the catalyst, but promoters such as dihydroacridine reactivate the system. Thermodynamic and kinetic analyses provide insight into the reaction mechanism, with Ni–H homolysis to generate a reactive hydrogen atom that itself acts as a hydrogen atom abstractor from ethers.

Acknowledgements
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Study of the depolymerization of polyethylene terephthalate (PET) organocatalyzed by imidazolium salts

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Polymers are essential to modern life, but their widespread use has generated significant environmental challenges associated with plastic waste accumulation.[1] Chemical recycling is a promising strategy for addressing this issue because it enables the recovery of valuable chemical building blocks.[2,3] Among common polymers, polyethylene terephthalate (PET) is particularly suitable for glycolysis, an efficient and relatively energy-saving chemical recycling process.[2,3] Catalysts derived from imidazolium salts represent an innovative alternative for this transformation. Their structural versatility enables their application in both homogeneous and heterogeneous catalytic systems, offering the potential to combine high catalytic activity and product yields with catalyst recovery and reuse, thereby contributing to more sustainable plastic waste recycling.[2,3] In this work, the glycolysis of waste PET bottles was investigated using imidazolium salts and their corresponding N-heterocyclic carbenes (NHCs) as catalysts. By varying the nitrogen substituents and the counteranion, the effects of steric factors and anion identity on the catalytic performance were systematically evaluated. The study included the synthesis and evaluation of imidazolium salts such as I*t*Oct·HCl, IMes·HCl, IPr*·HCl, IPr*^{OMe}·HCl, and IPr$^{\#}$·HCl, together with the corresponding NHCs derived from these precursors. The reaction conditions using the I*t*Oct·HCl catalyst were initially optimized through statistical response surface methodology using a Box–Behnken design (BBD). The optimization was performed under an ambient atmosphere using an ethylene glycol-to-PET molar ratio of 10:1, while temperature, catalyst loading, and reaction time were selected as the independent variables (Figure 1A). After determining the optimal conditions for the I*t*Oct·HCl system, a comparative screening of the other catalysts was performed. Among the systems investigated, IPr*^{OMe}·HCl exhibited the highest efficiency for BHET production (Figure 1B). Finally, the reaction mechanisms and corresponding energy profiles were investigated using DFT calculations.[4,5] The calculated energy values were consistent with the trends previously reported in the literature, providing further insight into the catalytic behavior of the investigated systems.[4,5]

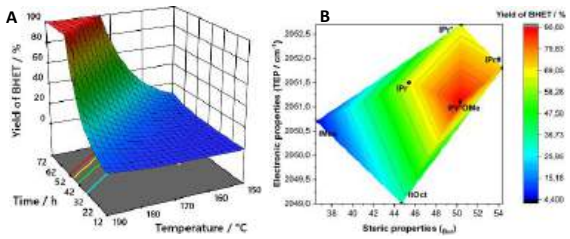

Figure 1. **(A)** Surface Model obtained through BBD analysis with ItOct·HCl. **(B)** Influence of electronic and steric properties in yield of BHET.

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New Modes of Transition Metal Reactivity with Boryl Pincers

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Tridentate "pincer" ligands are commonplace in the chemistry of transition metals. Our group is especially interested in the design of new polydentate ligands that encourage new types of reactivity at transition metal centers. We recently showed that rhodium and iridium complexes supported by a boryl/bis(phosphine) PBP pincer activate a variety of pyridines and other heterocycles selectively in the 2-CH ("ortho") position [1]. This robust and atypical selectivity is made possible by the participation of boron in these reaction as a Lewis acid towards the substrate. This presentation will explore the mechanisms of reactions relevant to this C-H activation, as well as of reactions that are important in the generation of active species, and some catalytic applications. Overall, the presentation will hope to show the uniqueness of a boryl moiety as a donor type in polydentate ligands.

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Base-Dependent Coordination Modes in Cp*iridium(III) Complexes Bearing Pyridine-Functionalized Triazenides

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This work reports the synthesis and characterization of four pyridine- and aryl-functionalized triazenes as precursors to organometallic iridium(III) complexes. The steric and electronic effects of different substituents on the aryl and pyridine groups were investigated to assess their influence on metal coordination. The ligands were characterized by ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectroscopy, whereas the resulting complexes were analyzed using 1D and 2D NMR spectroscopy and single-crystal X-ray diffraction.

The results demonstrate that the Brønsted base employed during triazenide anion formation is a key factor governing the coordination mode of the ligand. The use of a strong base favors the formation of a four-membered chelate through coordination of the terminal nitrogen atoms of the triazenide moiety, leaving the pyridine nitrogen uncoordinated. In contrast, using a weaker base, such as triethylamine, leads to a five-membered chelate via simultaneous coordination of the pyridine nitrogen and the central nitrogen atom of the triazenide group.

The change in coordination mode is evidenced in solution by NMR spectroscopy, particularly through changes in the chemical-shift of the pyridine *ipso* carbon attached to nitrogen [1]. In the solid state, single-crystal X-ray diffraction unambiguously confirms both coordination modes, demonstrating that synthetic conditions can control metal–ligand coordination and access distinct coordination isomers. The presence of an uncoordinated pyridine group in selected complexes makes these compounds attractive platforms for the development of potential catalysts [2].

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Abstract preparation

Design and synthesis of arylhydrazone-thioether based Pd-CNS pincer complexes with potential catalytic applications.

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In this work, a new family of unsymmetrical Pd-CNS pincer complexes based on tridentate arylhydrazone–thioether ligands were designed, synthesized, and characterized, with the aim of exploring their potential as catalytic precursors.

The synthetic approach was designed to provide a modular ligand framework in which the electronic properties of the arylthioether fragment could be modified through different para-substituents. Initially, a series of 1-[3-(4-*R*-phenylthio)-2-thienyl]ethanones (R = H, Me, Cl, NO_2) was synthesized through a nucleophilic substitution reaction between 2-acetyl-3-bromothiophene and the corresponding thiophenol, affording the desired ketones in good to excellent yields (63-88%). [1] These compounds were subsequently reacted with *N,N*-diphenylhydrazine to afford the corresponding tridentate arylhydrazone–thioether ligands in high yields (85–97%).

The resulting ligands were employed in direct cyclopalladation reactions with sodium tetrachloropalladate formed in situ from palladium (II) chloride in the presence of sodium chloride, affording four unsymmetrical Pd-CNS pincer complexes. The complexes were isolated as crystalline solids in yields ranging from 67 to 92% and displayed good stability toward air and moisture, with decomposition temperatures between 206 and 230°C. Structural characterization of the ketones, ligands, and cyclopalladated complexes was performed using infrared spectroscopy, ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy, mass spectrometry, and high-resolution mass spectrometry. The spectroscopic data supported the formation of the tridentate ligands and their subsequent cyclometalation, confirming the incorporation of the CNS coordination environment around the palladium center.

Overall, the results highlight the versatility of arylhydrazone–thioether ligands in the modular synthesis of unsymmetrical Pd-CNS pincer complexes. The structural features and stability of these complexes provide a basis for their further evaluation as palladium-based catalytic precursors, particularly in carbonylative cross-coupling reactions.

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LIGAND ASYMMETRY ENABLES CHARGE SEPARATION IN A ZWITTERIONIC TRI-ALUMINUM COMPLEX AND ITS THERMAL CONVERSION

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An unusual non-symmetric N-imidoylamidine–thioether–amine ligand was isolated and subsequently shown to stabilize a rare zwitterionic tri-aluminum complex upon reaction with trimethylaluminum.[1] Single-crystal X-ray diffraction, multinuclear NMR spectroscopy, and density functional theory (DFT) calculations reveal a charge-separated multinuclear framework in which a single asymmetric ligand simultaneously accommodates electron-rich and electron-deficient aluminum centers. This distinctive electronic structure highlights the ability of ligand asymmetry to induce significant polarization within multinuclear main-group complexes. Upon thermal treatment, the zwitterionic tri-aluminum species undergoes ligand fragmentation and methyl redistribution, leading to the formation of a neutral tetra-aluminum dimer featuring an unusual 16-membered macrocyclic framework. The structural rearrangement provides insight into the dynamic behavior of aluminum–ligand assemblies and demonstrates how ligand asymmetry can promote access to otherwise elusive multinuclear architectures. These results expand the structural diversity of zwitterionic aluminum chemistry beyond monometallic systems and establish ligand asymmetry as a useful design principle for controlling charge distribution and reactivity in multinuclear main-group complexes.

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Modeling of α-Olefin Polymerization Catalyzed by Transition Metals Using the Method of Moments and the Gamma Distribution

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A dynamic kinetic model for polyolefin production, coupling the Method of Moments (MoM) with the Gamma (Γ) distribution for MWD reconstruction, was developed for three systems: propylene/Ziegler-Natta (liquid-phase reactor), propylene/metallocene (gas-phase FBR), and ethylene/1-octene CCTP copolymerization (CSTR), solved with the implicit Radau method. Predictions agreed well with literature (Figure 1, Table 1): the Ziegler-Natta PDI stayed near the Flory limit from a fast/slow site balance; the metallocene system showed a broad PDI despite single-site kinetics (Mw error of only 0.53%), confirming the FBR residence time distribution controls dispersity; the CCTP system reproduced a narrow PDI via dormant-chain tracking. The MWD surfaces (Figure 1d–f) show the most probable chain length decreasing from Ziegler-Natta/metallocene toward CCTP, reflecting the different dispersity mechanisms [1–3].

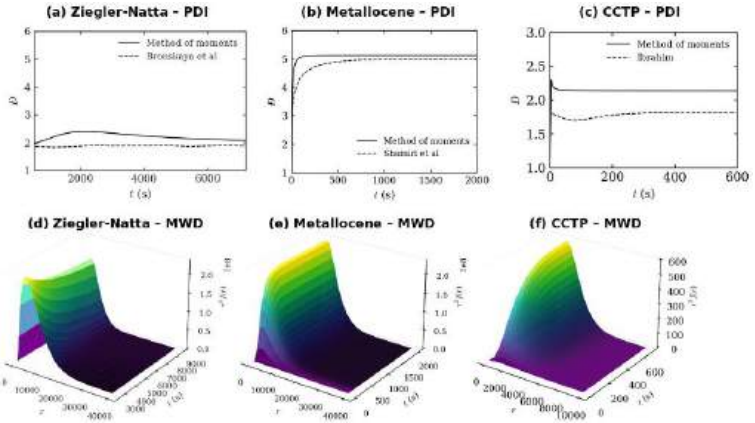

Figure 1. *(a–c) Predicted polydispersity index (D = Mw/Mn) versus time compared with literature: (a) Ziegler-Natta [4]; (b) metallocene, gas-phase FBR [2]; (c) CCTP, ethylene/1-octene [5]. (d–f) Corresponding molecular weight distribution (MWD) surfaces, $r^2 f(r)$ versus chain length r and time t, reconstructed via the Gamma distribution.*

Table 1. *Comparison of predicted and literature polydispersity index (PDI) and weight-average molecular weight (Mw) for the three catalytic systems studied.*

System	Model PDI	Lit. PDI	Error (%)	Model Mw (kg/mol)	Lit. Mw (kg/mol)	Error (%)
Ziegler-Natta	2.050	1.880	8.2	147.973	140.670	3.9
Metallocene (FBR)	5.129	4.983	2.84	139.196	143.486	0.53
CCTP	≈2.10	≈2.00	5.36	≈38.0	—	—

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SYNTHESIS AND REACTIVITY OF COBALT BIS(PHOSPHINIMINE) PINCER AND AZIDOPHOSPHONAMIDE COMPLEXES

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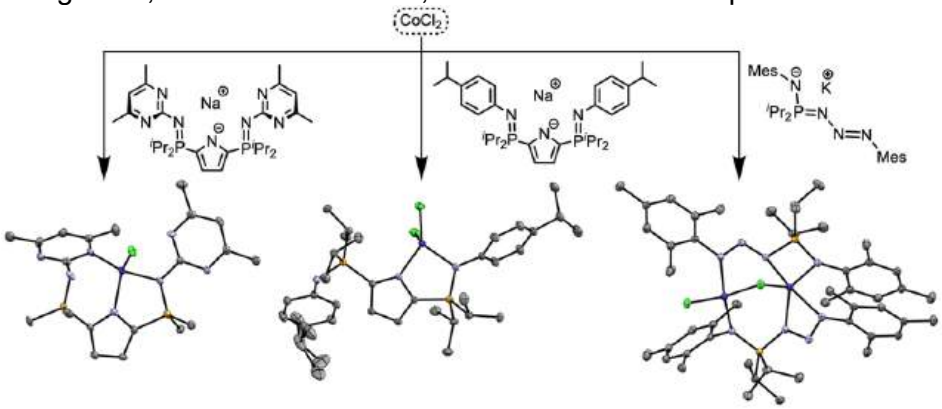
Sustainable chemical processes are vital for society's need for value-added chemicals. Despite this, many routes to fine chemicals are inefficient and produce vast quantities of waste. Thus, developing atom-economic methods is important to meet industrial demands and to establish a more sustainable future. The development of metal complexes which can serve as catalysts for various chemical transformations is therefore an important scientific activity. Precious metals, such as rhodium and iridium, have been traditionally used in fine chemical production because of their effectiveness in mediating numerous reactions (e.g., dehydrogenation, oxidative addition, etc.). However, such metals are expensive, highly toxic and negatively impact the environment.[1] In contrast, the smaller and less expensive group nine metal, cobalt, is more biologically tolerant and earth abundant.[1] However, its reaction chemistry is less predictable, largely due to its ability to undergo both one- and two-electron redox reactions. The Hayes group has previously developed synthetic protocols for generating families of monoanionic bis(phosphinimine) pincer and azidophosphonamide ligands, as well as the corresponding metal complexes thereof. Specific attention has been focused on rhodium and iridium complexes of ^{Ar}L and ^{Azido}L (^{Ar}L = 2,5-(^{i}Pr$_2$P=NAr)$_2$N(C$_4$H$_2$)$^-$; Ar = 4-^{i}PrC$_6$H$_4$ (^{Pipp}L), C$_4$H$_4$N$_2$ (^{pym}L); ^{Azido}L = ^{i}Pr$_2$P(N$_3$(Mes))N(Mes)$^-$; Mes = 2,4,6-Me$_3$C$_6$H$_2$).[2-6] This presentation will describe the synthesis, characterization, and reaction chemistry of cobalt bis(phosphinimine) pincer and azidophosphonamide complexes. Specifically, the diverse bonding modes and geometry, as well as the differences between cobalt and its heavy-metal congeners, rhodium and iridium, will be discussed in depth.



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Partial reduction of aromatic N-Heterocycles by heterobimetallic Pt-Ga complex

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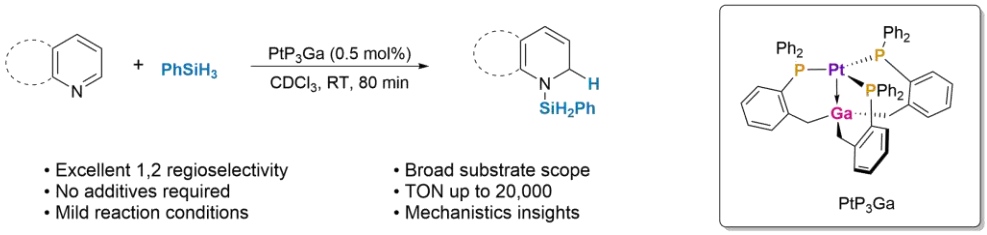

Partial dearomatization of N-Heterocycle compounds is a challenging transformation mainly due to the use of a highly pressurized combustible gas and the formation of different regioisomers that are difficult to separate. Hydrosilylation has emerged as a complementary strategy for the catalytic partial reduction of N-heterocycles, wherein the N-silylated product might act as a key intermediate for further functionalization. [1, 2]

Z-type ligands, such as Lewis acids (e.g. group 13 metal compounds), have risen as a promising tool for modulating the reactivity of transition metals (TM) in homogeneous catalysis. Motivated by this concept, we envisioned the incorporation of a Ga metalloligand into a Pt(0) complex would enable a TM → Z bonding interaction capable of tuning the TM electron density, unlocking new reactivity pathways. [3]

A bimetallic PtP_3Ga complex was synthesized and fully characterized. A Z-type interaction between Pt–Ga was supported by Natural Bond Orbital (NBO) analysis. This complex enables the catalytic 1,2-hydrosilylation of quinoline and pyridine derivatives with high efficiency and regioselectivity. The resulting catalytic system is applicable to a broad substrate scope and can operate with TON up to 20,000, providing streamlined access to synthetically valuable 1,2-dihydroheteroarene products.

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Sulfur-Enriched NHC Ligands: Bioinspired Platforms for Metal-Ligand Cooperativity and Redox Activity

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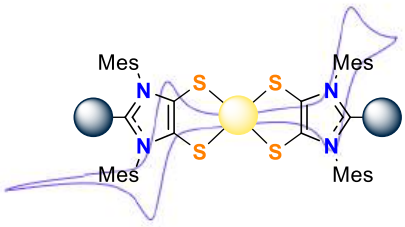
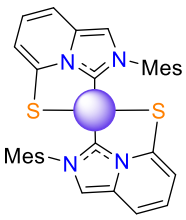
Sulfur donors play a fundamental role in biological metal centers, where they contribute to electron-transfer processes, redox regulation, and cooperative reactivity. Inspired by these natural systems, we have explored the incorporation of sulfur functionalities into N-Heterocyclic Carbene (NHC) ligands to generate electronically adaptive organometallic platforms.

This contribution will present two complementary approaches. The first involves the fusion of a dithiolene motif within an NHC backbone, affording an ambidentate ligand that combines the robust metal–carbene interaction with the rich redox chemistry of dithiolenes.[1] The second relies on a π-extended NHC-thiolate scaffold displaying non-innocent behavior[2] and supporting cooperative reactivity in transition-metal complexes.[3] Together, these examples demonstrate how sulfur-enriched NHC ligands provide access to new coordination modes, redox properties, and catalytic functions, opening attractive perspectives for the design of multifunctional organometallic systems.



dithiolene-backbone NHC



Bicyclic thiolate-NHC

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Synthesis and Characterization of New *fac*-[Re(CO)$_3$(N-N')X] Organometallic Compounds with Potential Anticancer Activity Bearing N-N' Ligands Derived from 2-Naphthaldehyde

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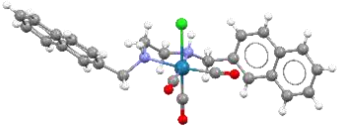
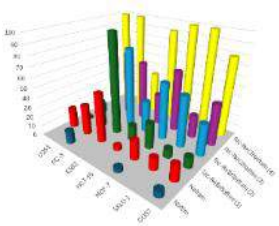
It is known that organometallic compounds containing the *fac*-[Re(CO)$_3$]$^+$ fragment exhibit high levels of thermodynamic and kinetic stability, alongside selectivity on cancerous cells and photophysical properties suitable for cell labeling. Furthermore, the coordination of nitrogenous ligands such as Schiff bases and their reduced derivatives coordinated to metallic centers enhance their biological activity, in some cases outperforming cisplatin. Inspired by these features, two nitrogenous ligands derived from 2-naphthaldehyde and a series of four rhenium(I) complexes were synthesized. The compounds were characterized by spectroscopic techniques and X-ray diffraction analysis. Biological evaluation across various cell lines revealed that complex *fac*-ReClNaftam exhibited potent inhibitory activity, although with low selectivity towards tumor cells, providing valuable insights for the future design of targeted rhenium-based anticancerogenic agents.



fac-ReClNaftam



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DESIGNER LIGANDS THAT INCORPORATE PHOSPHAZIDE AND AZIDOPHOSPHONAMIDE FUNCTIONALITIES

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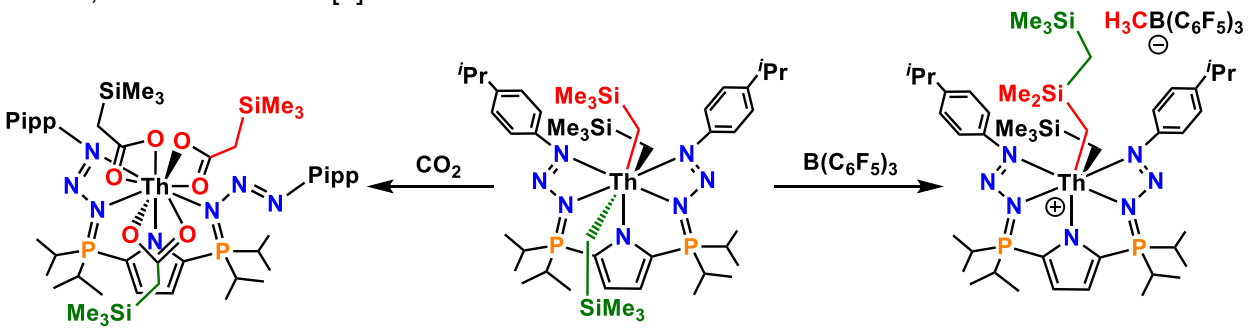
The Staudinger reaction,[1] wherein a tertiary phosphine is reacted with an organic azide, is a commonly utilized process to generate an iminophosphorane ($RN{=}PR_3$). Because they are prone to facile loss of N_2, the rarely observed phosphazide ($RN_3{=}PR_3$) intermediate is usually considered a fleeting species with limited synthetic value.[2] Nonetheless, several phosphazides, stabilized by hydrogen bonding, steric hindrance or metal coordination, have been serendipitously isolated.[3] In an effort to glean a deeper understanding of, and ascertain if, this functionality can serve to stabilize coordination and organometallic complexes, we designed several families of thermally robust mono- and diphosphazide, as well as related azidophosphonamide ($RN_3P{=}NR$), ligands.

The synthesis, reaction chemistry and thermal stability of actinide (U [4] and Th [5,6]) complexes supported by phosphazide scaffolds will be presented. Notably, divergent chemistry was observed for complexes supported by these phosphazide-containing ancillary ligands compared to their phosphinimine analogues, thereby suggesting that with judicious design phosphazides represent a viable functional group for coordination chemistry and homogenous catalysis. As proof of concept, a synthetic cycle of actinide-mediated CO_2 functionalization was established.[6] All aspects of these unique phosphazide-containing compounds will be discussed in detail. In addition, group 9 azidophosphonamide complexes, which exhibit unusual structures and bonding modes, will be described.[7]



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Re(I) and Ru(II) pH chemosensor based on amine imidazolphenanthroline

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Transition-metal complexes bearing imidazo-phenanthroline (**Ip**) derivatives are strategic platforms for the development of optical sensors. These contain functional groups that are sensitive to the presence of H^+ and OH^- ions, meaning the system's electronic properties depend on acid-base behavior. Based on the above, an interesting strategy is the use of photoactive complexes such as Re(I) and Ru(II) **Ip/polypyridyl derivatives**, which can serve as optical pH chemosensors. This study examines the effect of pH on the photophysical properties of both systems (**Fig. 1A**). Their acid-base behavior was evaluated using UV-Vis and fluorescence spectroscopic techniques. The UV-Vis studies of **ReIp-NH$_2$** showed a *bathochromic* shift in the absorption maxima accompanied by *colorimetric*changes as the pH was increased (**Fig. 1B**). On the other hand, in the luminescence studies, **RuIp-NH$_2$** exhibited the greatest changes, with *quenching* of the emission observed between 0.0 and 50.0 eq. of OH^- (**Fig. 1C**). Consistent with the above, the *batochromic* shifts in UV-Vis as well as the quenching of the photoluminescent response in both complexes were associated with the deprotonation of the NH group present in the Ip ligand. This process redistributes the electron density within the imidazole moiety ([**Re/RuIp -NH$_2$**]$^-$), which stabilizes the IL charge transfer and promotes photoinduced electron transfer (PET) from the deprotonated *imiphen* unit to the MLCT excited state of the complex (Ru(II) or Re(I)), which in turn leads to the deactivation of the ^{3}MLCT transition.

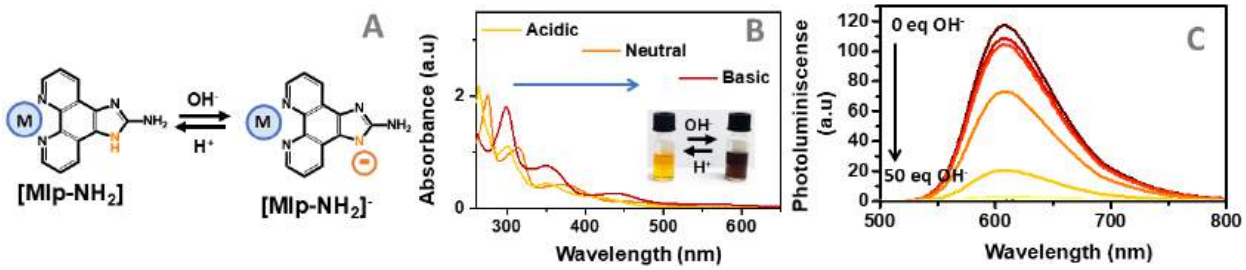

Fig.1. [M] = $ReBr(CO)_3$, $[Ru(bpy)_2]^{2+}$ (A). UV-Vis spectra of $ReIpNH_2$ (25 uM, 3:97 DMSO:Water) (B). Photoluminescent spectra of $RuIpNH_2$ (25 µM, 1:9 ACN:Water, λ_{exc} 461 nm) (C).

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Ag(I) COMPLEX WITH PIPERONAL-N(4)-METHYLTHIOSEMICARBAZONE: SYNTHESIS, CHARACTERIZATION AND IN VITRO ANTIBACTERIAL ACTIVITY AGAINST *S. AUREUS* AND *E. COLI*

Edwin Briñez-Ortega[1], Ana Esperanza Burgos Castellanos[1], Yosimayrobi Endo Navarro[1]

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In this work, the complex $[Ag(L)_2]NO_3$ was synthesized, where L corresponds to the piperonal-N(4)-methylthiosemicarbazone ligand, for the purpose of evaluating its in vitro antimicrobial activity against *S. aureus* and *E. coli* by the agar well diffusion method [1]. The ligand L was obtained by the condensation reaction between piperonal and 4-methyl-3-thiosemicarbazide, under reflux for 4 h. The silver(I) complex was synthesized by a stoichiometric ligand:metal 2:1 reaction in ethanol under dark and reflux conditions for 24 h. The resulting grayish precipitate was filtered and washed with small volumes of ethanol.

The structural characterization of the $[Ag(L)_2]NO_3$ complex was performed by comparing the IR spectra of the free ligand and the complex. The results indicated that L coordinates bidentately to the Ag(I) metal center as a thione tautomer through the sulfur donor atoms of the thiocarbonyl group (S) and the azomethine nitrogen (N). This coordination was evidenced by the shift of the band attributed to ν(C=S) from 1102 cm^{-1} in the ligand to 1259 cm^{-1} in the complex, as well as by the shift of the band corresponding to ν(-CH=N⁻) from 1584 cm^{-1} to 1591 cm^{-1}. Additionally, the formation of the Ag-S and Ag-N bonds was confirmed by the presence of bands at 563 and 808 cm^{-1}, respectively. The characterization of the synthesized compounds was complemented by elemental analysis (CHN), determination of melting point, molar conductivity, among other techniques.

Finally, the $[Ag(L)_2]NO_3$ complex, evaluated in DMSO, showed a minimum inhibitory concentration (MIC) of 0.250 $mg{\cdot}mL^{-1}$ against both bacterial strains, *S. aureus* (Gram-positive) and *E. coli* (Gram-negative). No differences in antibacterial activity were observed related to the structural characteristics of the cell wall of either bacterium. The antibacterial activity of the complex could be attributed, in part, to its greater lipophilic nature as a consequence of metal coordination, according to Tweedy's chelation theory, which would favor its permeation through the cell membrane and, subsequently, its interaction with intracellular active sites, interfering with metabolic processes essential for the growth and survival of microorganisms [3].

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STRUCTURAL AND CHEMICAL RESEARCH ON BIOMACROMOLECULES WITH SPECIFIC FLUORESCENT LIGANDS, WITH APPLICATIONS IN NEUROCHEMISTRY, OPTOGENETICS, AND DRUGS DESIGN.

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Human transferrin (Tf) is a glycoprotein with a molecular weight of around 80kDa, which is present in blood plasma. Its function is to transport iron from its site of absorption to all cells via the blood vessels. Iron transport by transferrin is mediated by the transferrin receptor (TfR), a 97kDa protein expressed as a homodimer at the cell surface. It circulates in the bloodstream at a pH of 7.4 until it binds to the TfR, forming a macromolecular complex that is internalised by endocytosis to form an endosome with a pH of 5.4, which is more acidic than that of the blood. The TfR is expressed in cells that comprise the blood–brain barrier (BBB). Only molecules that are specific to the functions of the central nervous system (CNS) can enter the CNS via this barrier by transmembrane diffusion, provided they meet certain physicochemical criteria such as low molecular weight and high lipid solubility. Alternatively, human transferrins can enter through processes regulated by specific receptors. However, the treatment of certain neurological diseases is hindered by the BBB's restriction on drug passage. The aim of this research is use the human transferrins as an specific drug's transporter to the brain via our suggested strategy called Troyan's horse.

On the other hand, phototropins are a group of photoreceptors that play a crucial role in light-dependent plant responses. They are highly sensitive to blue light and trigger a series of cellular responses that ensure the plant's survival. In the plant Arabidopsis thaliana, two phototropin isoforms, Photo1 and Photo2, have been identified. Consisting of approximately 996 and 915 amino acids, respectively, Photo1 and Photo2 share about 86% sequence homology. Each phototropin has a photosensitive domain at the N-terminus and an effector domain at the C-terminus, which consists of a kinase domain. The photosensor domain, on the other hand, is composed of two LOV (light-oxygen-voltage) domains: LOV1 and LOV2. The study of photosensitive domains, particularly light-sensitive ones such as LOV, has gained significant relevance in recent years due to their growing applications. One of this applications is shown on this talk, using the same Troyan's horse strategy, but using a zebra fish as a biomedical model to follow the pathway to the brain thoughout applying a blue light in order to follow the specific drugs against glioblastoma in the brain, which is one of the most dangerous diseases nowadays in the brain's cancer.

Acknowledgements: The authors thanks to the DGAPA Project **PAPIIT No. IN206125** for supporting this research.

Counteranion-Controlled Antimicrobial Activity in Cationic Pd(II)–Phenanthroline Complexes

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The development of metal-based antimicrobials has emerged as a promising strategy to combat antimicrobial resistance, with Pd(II) complexes attracting increasing attention due to their versatile coordination chemistry and tunable biological properties [1]. While extensive efforts have focused on ligand design, the influence of counteranions on the biological activity of cationic metal complexes remains comparatively underexplored, despite their potential to modulate physicochemical properties through second-sphere interactions.

Herein, we report a systematic investigation of the effect of counteranion identity on the antimicrobial activity of a family of cationic bis(1,10-phenanthroline)palladium(II) complexes bearing BF_4^-, PF_6^-, and OTf^- counteranions. Although all complexes possess an identical PdN_4 primary coordination environment, pronounced differences in biological activity were observed. The PF_6^- and BF_4^- derivatives exhibited the highest antibacterial activity against Gram-positive bacteria, with minimum inhibitory concentration (MIC) values as low as 12.5 μg mL^{-1}, whereas the OTf^- analogue showed substantially lower activity (MIC = 200–400 μg mL^{-1}). Similar trends were observed against *Candida albicans*, highlighting a clear dependence of antimicrobial efficacy on the identity of the counteranion.

The observed activity trends are consistent with differences in ion pairing and associated physicochemical properties arising from second-sphere interactions [2]. These findings highlight that counteranions are not merely spectator ions but can significantly influence the biological behavior of cationic Pd(II) complexes. More broadly, this work identifies counteranion exchange as a simple and effective strategy for tuning the physicochemical and antimicrobial properties of metal-based complexes without modifying their primary coordination sphere.

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BIOINSPIRED COPPER(II) COMPLEXES FOR OXIDATIVE CLEAVAGE OF RECALCITRANT POLYSACCHARIDES

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The biocatalytic breakdown of recalcitrant polysaccharides is key for both environmental remediation and the use as renewable feedstocks for the sustainable production of biofuels, chemicals, and materials [1,2]. This project addresses this challenge through the design and synthesis of copper coordination compounds bioinspired by the active site of LPMO enzymes, natural catalysts used by microorganisms specialized in lignocellulose degradation. These enzymes are particularly notable for their ability to oxidize strong C–H bonds (>95 kcal/mol) [3], a key step that initiates the cleavage of glycosidic bonds at the C1 or C4 positions of long-chain crystalline polysaccharides.

The copper complexes proposed for this project mimic the LPMO active site through the incorporation of mixed nitrogen-donor atoms from pyridine and benzimidazole groups, simulating the natural histidine brace [4]. Their specific structural and electronic properties are anticipated to promote the degradation of their natural substrates such as chitin and cellulose and potentially be extended to sargassum [5].

Finally, it is important to note that the mechanism of LPMOs remains unclear. While several reaction intermediates have been proposed, a definitive mechanism has yet to be established [6]. Therefore, this project aims to design experiments to identify the reaction intermediates formed and, with the aid of DFT calculations, propose a suitable reaction mechanism.

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Synthesis, characterization and evaluation of the biological activity of new Cu(II) and Ag(I) complexes from a thiosemicarbazide type ligand derived from caffeine.

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Bacterial infections and cancer remain among the leading causes of morbidity and mortality worldwide, and the rise of multidrug-resistant bacteria together with the limitations of current chemotherapeutic agents highlights the need for new therapeutic candidates with improved efficacy and reduced toxicity.[1,2] Medicinal inorganic chemistry, which incorporates transition metals into bioactive organic scaffolds to broaden their mechanisms of action, offers a promising strategy to address this need.

In this work, caffeine was used as a molecular platform for the design of a novel thiosemicarbazide derivative,[1–3] exploiting the strong metal-chelating capacity conferred by the nitrogen and sulfur donor atoms of the thiosemicarbazide moiety.[4] The organic ligand was synthesized through structural modification of caffeine, and preliminary spectroscopic evidence supports the successful incorporation of the thiosemicarbazide group into the caffeine scaffold; full structural characterization is currently in progress. This ligand will subsequently be used to obtain coordination complexes with Cu(II) and Ag(I), two metal centers widely recognized for their ability to potentiate the biological activity of thiosemicarbazide-based ligands through mechanisms such as oxidative stress induction, metalloenzyme inhibition and enhanced interaction with cellular targets.[5,6]

The resulting complexes are expected to display improved antimicrobial and antitumor activity relative to the free ligand, consistent with previous reports on related caffeine-thiosemicarbazide and metal-thiosemicarbazide systems.[7,8] This work is therefore expected to provide new structure-activity insights at the interface of caffeine chemistry, thiosemicarbazide coordination chemistry and medicinal inorganic chemistry, contributing to the search for more effective, lower-toxicity therapeutic agents against bacterial infections and cancer.

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BIOMASS VALORIZATION WITH IRON AND COPPER

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Inspired by copper-dependent Lytic Polysaccharide MonoOxygenase enzymes (LPMO) [1,2], we used synthetic systems based on the "histidine brace" motif to test their activity in the oxidative degradation of recalcitrant biomass. This includes the model substrates *p*-nitrophenyl-β-D-glucopyranoside and cellobiose, as well as cellulose and bagasse from agave plants [3,4]. We extended this work to iron as a more economically viable option, based on its redox chemistry and potential for organic substrate oxidations. Bagasse degradation to water-soluble products reaches 80% with most iron and copper complexes, as well as with simple metal salts. The best conditions for degradation are at a controlled pH between 5-6. Further extension of this chemistry to the degradation of dry sargassum biomass afforded similar results, presenting an opportunity for the valorization of a contaminant in Caribbean beaches [5]. Finally, identification of soluble products by comparison of HPLC retention times with authentic samples allowed the identification of glucose and gluconic acid in the case of cellulose, and the same products along with yet unidentified products in the case of sargassum-based alginic acid.

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Mo Complexes with Thioether Functionalized N-heterocyclic Carbene Ligands Inspired by the Active Site of Mo-Nitrogenase

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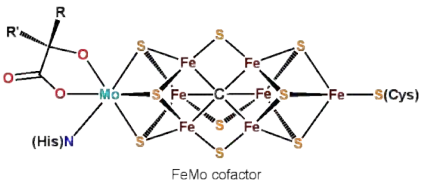
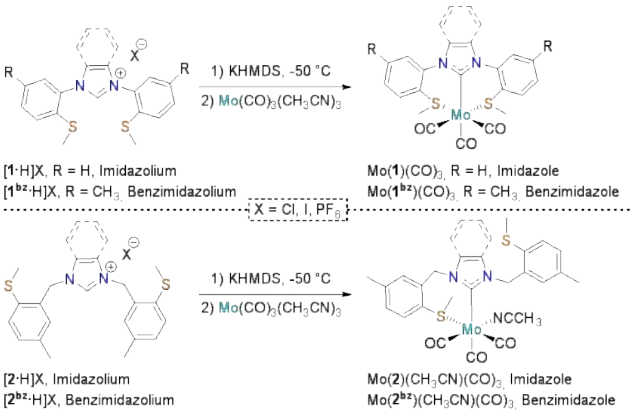
To ensure sufficient food supplies for the rapidly increasing world population ammonia plays a key role, since around 80% of the global ammonia production is used in the agricultural sector for the production of fertilizers.[1] Industrially, ammonia is produced *via* the Haber-Bosch process which reduces N_2 using H_2 from fossil fuel origin in the presence of a heterogeneous Fe catalyst under very high pressure and temperature. In nature, Nitrogenases can reduce atmospheric N_2 effectively under mild conditions without the need of H_2. In order to reduce energy demands and become independent from fossil fuels, it is important to design and study model compounds inspired by the active sites of nitrogenases. Since Mo-Nitrogenase is the most efficient one regarding N_2 reduction we herein focus on its active site, the FeMo cofactor (structure on the right).[2]



FeMo cofactor

We designed four thioether functionalized NHC ligands based on imidazole (**1**, **2**) and benzimidazole (**1**^{bz}, **2**^{bz}) and obtained the corresponding Mo(0) complexes using *fac*-$Mo(CO)_3(CH_3CN)_3$ as a precursor. Single crystal X-ray analysis revealed Mo complexes where only one sulfur coordinates when a CH_2 group is present between the (benz)imidazole and the thioether moieties. However, Mo-SCS complexes could be obtained using ligands which lack the CH_2 groups. With these four Mo(0) complexes in hand we are currently studying their reactivity, the removal of the carbonyl ligands, and their ability to coordinate N_2.



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Copper (II) - Neocuproine ternary complexes: uncommon structures derived from unusual ligand assembly and their biological implications

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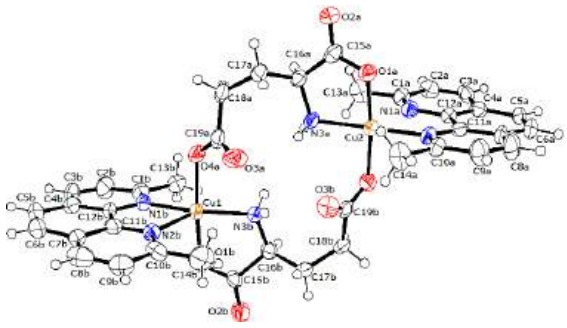
The family of diimine-type copper (II) ternary complexes is a vast collection of molecules that includes more than 9,000 crystallographic reports [1]. This interest is largely explained by their proven anticancer properties [2]. Although this same type of ternary complex shares a general structure, there are cases in which this rule is fulfilled in highly unusual ways. In this work, we present five neocuproine-copper(II) ternary complexes, which exhibit structural peculiarities with respect to the family of mixed complexes. All of the above is part of our study on the relationship between structure secondary ligands and the complex biological activity



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CoNPs Supported on Tetramethylguanidine-Functionalized Halloysite Nanotubes for Alkoxy- and Aminocarbonylation

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Carbonylative reactions are atom-efficient methods for synthesizing esters and amides from aryl halides, providing access to valuable carbonyl-containing compounds used in pharmaceuticals and fine chemicals.[1,2] While palladium catalysts dominate these transformations, the development of sustainable alternatives based on earth-abundant metals such as cobalt is highly desirable.[3,4] In this work, halloysite nanotubes (HNTs) functionalized with tetramethylguanidine (TMG) were employed as supports for cobalt nanoparticles to promote alkoxy- and aminocarbonylation reactions. Successful HNT functionalization was confirmed by DRIFTS and solid-state ^{13}C and ^{29}Si NMR spectroscopy, which evidenced the presence of TMG linked to Si without altering the aluminosilicate structure. CoNPs were subsequently deposited through decomposition of $Co_2(CO)_8$ under hydrogen, yielding **CoNPs@HNTs/TMG** while preserving the nanotubular architecture. HAADF-STEM analysis revealed well-dispersed spherical nanoparticles with an average diameter of 3.56 ± 0.51 nm, significantly smaller than those obtained on non-functionalized HNTs (10.07 ± 2.73 nm), highlighting the role of TMG in controlling particle growth. **CoNPs@HNTs/TMG** exhibited superior activity to non-functionalized CoNPs@HNTs in the alkoxy- and aminocarbonylation of aryl iodides. Under relatively mild conditions, the catalyst afforded esters and amides with excellent selectivity and moderate to good yields. The catalyst was recyclable for six runs without detectable cobalt leaching, representing one of the first supported cobalt nanoparticle systems reported for these carbonylation reactions.

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Electronic Basis of Iron-Sulfur Cluster Reactivity

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I will describe my research group's use of synthetic iron-sulfur clusters to understand the properties and reactivity patterns of iron-sulfur proteins. Emphasis will be placed on (i) synthetic methods for introducing strong-field ligands into a cluster's coordination sphere, and (ii) connecting iron-sulfur clusters' electronic properties with their reactivity and biological function.

OXIDATIVE COUPLING OF 2,6-DIMETHYLPHENOL CATALYZED BY BIOINSPIRED COPPER COMPLEXES

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Polyphenylene oxide (PPO) is a significant thermoplastic primarily synthesized by oxidative coupling of 2,6-dimethylphenol (2,6-DMP). Metal ion complexes that catalyze this reaction have been widely studied.[1] Comparative studies of bioinspired copper complexes have shown that structural differences directly affect the catalytic efficiency.[2, 3]

In this work, the catalytic capacity of four imidazole-derived ligands in the oxidative coupling of 2,6-DMP is studied. The polymer obtained was analyzed by high-performance size-exclusion chromatography (HPSEC) to compare the effect of the catalyst on the molecular weight and, thereby, total chain length.

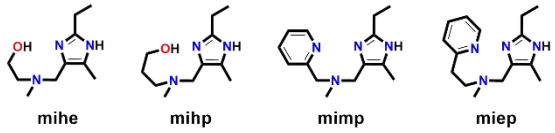

Figure 1. Bioinspired ligands derived from imidazole.

UV-Vis spectroscopy, determination of stability constants, and electrochemical studies were performed to propose a catalyst regeneration model. Density Functional Theory (DFT) M06/6-31+G(d,p) calculations support the model.

Catalyst	Yield (%)	Mn	Mw	Total Chain Length
Cu*mihe*	75.52	6857	15599	130
Cu*mihp*	68.32	6473	13012	108
Cu*mimp*	51.51	6368	13982	116
Cu*miep*	47.49	4975	12475	104

Table 1. Yield and HPSEC results.

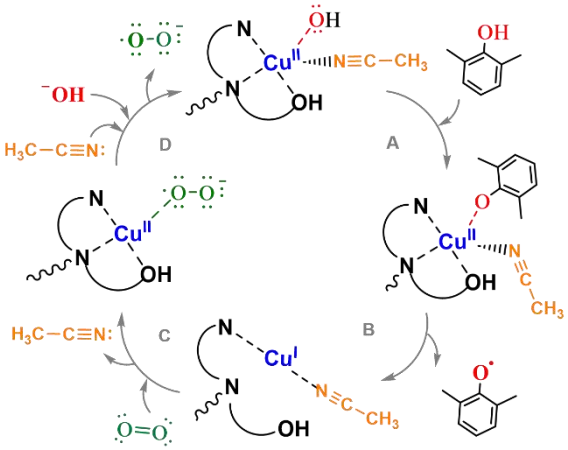

Figure 2. Catalyst regeneration model proposed.

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