



Facultad de Ciencias y Tecnologías Químicas
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Comité editorial: Abelardo Sánchez, Alba Escalona, Beatriz García-Béjar, Rafael Granados, Antonio de la Hoz, José Pérez.

PRESENTACIÓN

Como todos los años el número de este mes es monográfico y está dedicado a la decimosexta edición del simposio "Ciencia Joven". Se incluye también una referencia al acto realizado sobre el cambio de nombre del edificio de laboratorios que se dedicará a la Dra. Margarita Salas.

El comité editorial.

La Facultad de Químicas de la UCLM celebra su XVI Simposio de Ciencia Joven



La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha ha inaugurado su ya tradicional Simposio de Ciencia Joven que reúne a más de 120 jóvenes investigadores con el objetivo de poner en común sus líneas de trabajos y darlas a conocer a la sociedad. En el mismo, se ha disfrutado de las ponencias de varios expertos, entre ellos la de la directora del Centro Nacional de Investigaciones Oncológicas (CNIO), María Blasco, quien ha sido la encargada de descubrir la placa con la que se renombra al edificio de laboratorios de la Facultad de Químicas, que pasa a denominarse Margarita Salas.

Los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas en el Campus de Ciudad Real de la Universidad de Castilla-La Mancha (UCLM) presentan a la comunidad académica sus líneas y resultados de investigación con motivo de la celebración del XVI Simposio Ciencia Joven, una iniciativa científica y formativa que pretende promover y divulgar la investigación realizada por los jóvenes en los campos científicos y tecnológicos relacionados con la Química, la Ingeniería Química y la Ciencia y Tecnología de los Alimentos, enseñanzas tradicionales del centro, y acercar su trabajo a la sociedad.

Más de 120 jóvenes participan en esta iniciativa que ha inaugurado el rector de la UCLM, Julián Garde, y que edición tras edición adquiere más relevancia como así lo demuestra el hecho de que en la misma participen en su mayoría investigadores de la Facultad de Ciencias y Tecnologías Química, como organizadora del evento, pero también de otros centros y campus de la propia institución académica.

Garde, que ha felicitado a la organización por esta “magnífica” iniciativa, lo cual queda refrendado “por la calidad de su programa”, ha apuntado que la Facultad de Ciencias y Tecnologías Químicas es “uno de los centros por excelencia” de la UCLM, y ha indicado que una de las “señas de identidad” del equipo de Gobierno de la institución académica es “apoyar la investigación con fondos”.

INAUGURACIÓN

De su lado, el decano de la Facultad de Ciencias y Tecnologías Químicas, Manuel Andrés Rodrigo, ha explicado que ésta es una de las “múltiples” actividades que celebra el centro para acercar la ciencia a la sociedad y ha añadido que con ésta en concreto, además, se pretende que los jóvenes investigadores aprendan a organizar actividades científicas, ya que es una parte más de su formación.

Asimismo, el decano se ha referido a que son muy variadas las líneas de investigación que se presentarán en este simposio y van desde las relacionadas con la Química, la Ingeniería Química y la Tecnología de Alimentos que pueden cursarse en el propio centro, a otras que tienen que ver con la energía o el desarrollo de materiales, y todo ello aplicado a las empresas. “Somos un centro con 35 grupos de investigación activos y canalizamos proyectos de investigación por valor de 8 millones de euros”, ha dicho.

Junto al rector de la UCLM y al decano de la Facultad de Ciencias y Tecnologías Químicas, en la inauguración del simposio ha participado su organizadora, la profesora María Antonia Herrero, quien ha asegurado que esta es una actividad “por y para los estudiantes de doctorado”; el director general de Universidades, Investigación e Innovación de la Junta de Comunidades de Castilla-La Mancha, Ricardo Cuevas, quien ha trasladado el apoyo del Gobierno autonómico al talento joven de la región; y el presidente de la Unión Internacional de Química Pura y Aplicada (IUPAC), Javier García-Martínez, quien ha afirmado que son los jóvenes investigadores los que “aportan soluciones a los problemas actuales”.

En este encuentro tendrán cabida 35 comunicaciones orales de noveles investigadores, 41 comunicaciones flash virtuales de vídeos de unos tres minutos de duración que pueden verse en las redes sociales de la Facultad de Ciencias y Tecnologías Químicas, y ponencias de expertos invitados como la del propio presidente de la IUPAC o de la directora del Centro Nacional de Investigaciones Oncológicas (CNIO), María Blasco.

Gabinete de Comunicación UCLM. Ciudad Real, 22 de junio de 2022

Edificio Margarita Salas



El edificio Francisco Fernández Iparraguirre de la Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en el Campus de Ciudad Real cambia hoy su nombre y toma el de la ya fallecida bioquímica española Margarita Salas. Su discípula María Blasco, una de las científicas españolas más reconocidas internacionalmente por sus contribuciones fundamentales sobre los telómeros y la telomerasa ante la función que desempeñan en el cáncer y el envejecimiento, ha sido la encargada de descubrir la placa de rebautizo de este edificio que alberga laboratorios docentes y de investigación y las áreas de Matemáticas, Física, Organización Industrial, Expresión Gráfica y Geología.

El decano de la Facultad de Ciencias y Tecnologías Químicas de la UCLM, Manuel Andrés Rodrigo, ha justificado este cambio de nomenclatura para ofrecer “referentes científicos de verdad” a la sociedad, en general; y a los estudiantes del centro, en particular. Rodrigo ha recordado que Margarita Salas fue la investigadora química “más relevante” de toda la historia de nuestro país, y ha subrayado que “no sólo es un referente, sino que es un referente femenino, un dato a destacar si tenemos en cuenta que el 60 % de los estudiantes de nuestra Facultad son mujeres”.

A este acto también ha asistido el rector y algunos miembros del equipo de Gobierno de la UCLM, Ricardo Cuevas, representantes del Ayuntamiento de Ciudad Real y numerosos profesores y estudiantes de la Facultad de Ciencias y Tecnologías Químicas.

Gabinete de Comunicación UCLM. Ciudad Real, 22 de junio de 2022



Dr. Javier García Martínez

Química circular: Cómo construir una nueva economía a escala molecular



Los fondos europeos de recuperación han puesto el foco y los recursos en la economía circular. Hoy se reciclan, con mayor o menor éxito, todo tipo de materiales. Sin embargo, en la mayoría de los casos, reciclar significa simplemente recoger, separar y conformar de nuevo. Obviamente, este proceso tiene limitaciones importantes porque, tras sucesivos ciclos, cada vez se hace más difícil dar nueva vida a los residuos debido a la acumulación de impurezas y a la pérdida de propiedades. Para facilitar el reciclado, utilizamos distintos contenedores para separar los residuos, existen puntos de recogida y se conceden ayudas públicas; sin embargo, hemos hecho muy poco para diseñar materiales que nos faciliten su transformación. A pesar de los años que llevamos reciclando, los materiales que queremos reutilizar hoy son muy parecidos a los que tirábamos ayer. Por eso su reciclaje resulta tan difícil y buena parte de lo que se recoge termina finalmente en el vertedero. Parece lógico rediseñar estos materiales para que su transformación sea lo más sencilla posible.

Para que la economía circular pueda girar sin fin y hacer realidad su objetivo de reutilizar continuamente lo que producimos, es necesario repensar el reciclaje. La química circular consiste en rediseñar los procesos y los materiales para que desde su concepción estén diseñados de forma que su recuperación, separación y reconversión en materia prima sean lo más sencillo, eficiente y rentable posible.

Un buen ejemplo de lo que podemos conseguir mediante el diseño molecular de la economía circular lo constituye una nueva generación de plásticos que incluyen en su estructura enlaces que pueden romperse fácilmente. De esta manera, es posible recuperar los monómeros que los constituyen y así asegurar su reutilización. Hace apenas unos meses, investigadores de la universidad de Constanza en Alemania, publicaron en la revista Nature un nuevo tipo de plásticos que pueden recuperarse y reutilizarse de forma casi indefinida. Este logro ha sido posible gracias a la incorporación en su estructura de puntos de ruptura que permiten desensamblarlos fácilmente en sus componentes básicos. De forma similar, otros investigadores, en este caso de la universidad de Berkeley, utilizan enlaces dinámicos para producir termoplásticos. Estos enlaces permiten componer y descomponer estos materiales de forma reversible y virtualmente indefinida, lo que facilita que su recuperación y

hace más sencillo y rentable recuperar y reutilizar todo lo que producimos. No hay mejor ejemplo de lo que digo que los recientes avances en el uso de CO_2 como materia prima para producir plásticos, combustibles e incluso materiales avanzados. Investigadores de la universidad de Toronto han logrado convertir el CO_2 en etileno, que es el compuesto con el que fabricamos algunos de los plásticos más comunes. Para ello han utilizado corriente eléctrica procedente de fuentes renovables. Gracias a la luz solar es posible eliminar el CO_2 de la atmósfera y transformarlo en todo tipo de materiales, combustibles y productos químicos de alto valor añadido. Hace apenas unas semanas, un equipo de investigadores japoneses y norteamericanos, han mejorado este proceso logrando eficiencias cercanas al 90% de transformación de CO_2 en etileno. Estos y otros avances similares posibilitan la generación de emisiones negativas de CO_2 , que tienen un papel muy importante en la descarbonización nuestra economía. La química circular nos permite transformar un residuo en un recurso, contribuyendo así a la lucha contra el cambio climático.

Otro de los gases que van a jugar un papel muy importante en la transición energética es el hidrógeno. Desde hace décadas, se ha propuesto el uso de esta alternativa a los hidrocarburos como combustible renovable ya que su combustión genera únicamente agua, en lo que constituye un excelente ejemplo de economía circular en el sector energético. El problema es que en la actualidad para generar hidrógeno es necesario utilizar combustibles fósiles. Sin embargo, en los últimos años se han producido avances muy notables para producir hidrógeno directamente del agua utilizando, no combustibles fósiles y altas temperaturas, sino corriente eléctrica a temperatura ambiente. Estos avances, combinados con el abaratamiento y disponibilidad de las energías renovables, ha vuelto a poner al hidrógeno en el foco de atención de la industria. De hecho, es una de las grandes apuestas de los Fondos Europeos de Recuperación con más de 500 proyectos presentados. Grandes empresas españolas como Iberdrola, Enagás, Endesa, Repsol, Naturgy, Acciona, Talgo o CAF, conscientes de la oportunidad, ya han comprometido fuertes inversiones para liderar esta nueva industria basada en el hidrógeno verde.

La economía, de algún modo también circular, de nuestro país es en buena parte solar. El buen tiempo que nos acompaña casi todo el año es una de las razones por las que millones de personas nos visitan. Por otra parte, el sol genera buena parte de la electricidad que utilizamos. Nuestro país puede aprovechar la ventaja competitiva que nos da nuestra posición geográfica para generar energía renovable de forma muy competitiva. Vender electrones verdes a buen precio es sin duda una excelente inversión, pero resulta mucho más rentable vender moléculas. Avanzar en la cadena de producción desde el modesto electrón a compuestos químicos de alto valor añadido no solo es una inversión rentable sino un paso importante hacia una economía más sostenible, resiliente y competitiva construida a escala molecular.

Javier García Martínez

Presidente de la Unión Internacional de Química Pura y Aplicada.

Presidente de la Academia Joven de España.

Catedrático de Química Inorgánica de la Universidad de Alicante y Catedrático de la Fundación Rafael del Pino.

Patrono de la Fundación Gadea por la Ciencia.

Dr. Ricardo Cuevas

Consejería de Educación, Cultura y Deporte

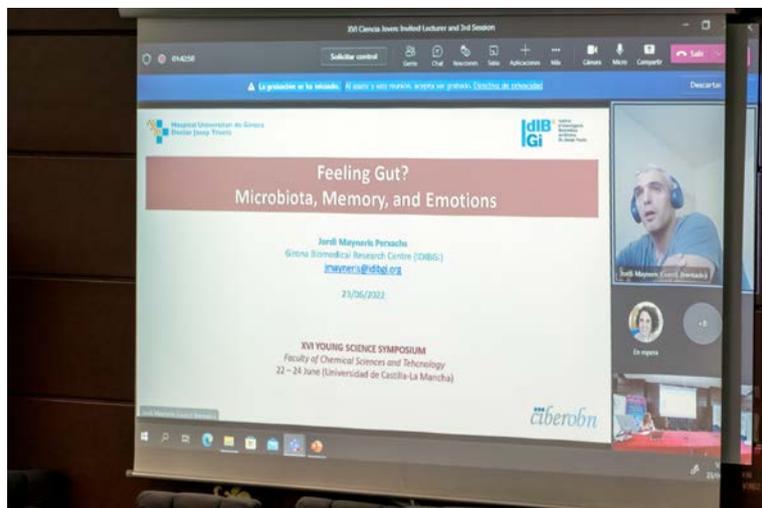


Dra. María Blasco

Understanding Aging to Cure Diseases



Dr. Jordi Mayneris Perxachs Feeling Gut? Microbiota, Memory, and Emotions



Dr. Jordi Mayneris-Perxachs holds two BSc in Chemistry and Food Science and Nutrition and a PhD in Theoretical and Computational Chemistry. He is an expert in Systems Biology and Omics Sciences, particularly metabolomics, metagenomics and transcriptomics.

He acquired most of this expertise during a four-year postdoctoral stay (2011-2015) at the University of Reading and Imperial College London (UK) under a Marie Curie COFUND program. There, he pioneered the description of gut microbial-derived alterations in Tryptophan metabolism with undernutrition and environmental enteropathy applying a metabolomic approach. In 2015, he was granted a Marie Curie fellowship (Tecniospring program) to join the Units of Nutrition and Omics Science at the Technology Centre of Catalonia (EURECAT).

In 2019, he was granted a Miguel Servet (ISCIII) and joined the Girona Biomedical Research Institute (IDIBGI), where he leads the Integrative Systems Medicine research. He applies cutting edge post-genomic technologies combined with advanced computational techniques (i.e., machine learning) in large human cohorts and pre-clinical models to obtain a holistic view of the holobiont and unravel the molecular mechanisms underlying the pathogenesis of cardiometabolic disease and cognitive performance, with particular emphasis on the complex microbiome-host interplay.

He has led the discovery of microbial profiles and functional signatures linked to memory, inhibitory control, depression and fatty liver, publishing the results in high-impact journals such as *Cell Metabolism* (IF=27.287), *Gut* (IF=23.059), *Cell Host & Microbe* (IF=21.023) and *Microbiome* (IF=14.652).

Dr. Daniel T. Peters

A journey through the valley of death: commercialization of academic research from the perspective of a post-doc

The “Valley of Death” is a term used to describe the gap between research and its successful commercial application. The challenges involved in this process are immense, and the failure rate of new start-up companies is high. It can be especially daunting for early career researchers, who have often spent many years training to do specialist research, to consider the new skills and mindset needed to develop a successful business. However, there is a great overlap between the skills required by an entrepreneur and those possessed by an early career researcher. Government and industry have also developed programmes and mentorship networks to help researchers transition from academia to business to commercialise their technologies and drive innovation. Finally, as competition for permanent academic positions intensifies, the spin out route can provide an attractive alternative for scientists who are keen to continue their research and make an impact on the wider world.

In this talk, I will describe my experience so far of the journey towards forming a spin-out company and how, as a post-doc, I have begun learning the required skills, including the importance of understanding and identifying the commercial value of a technology, the advantages of market discovery and training programmes, and the benefits of social media for building networks.

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Dr. Raquel Reina I+D+i en INCARLOPSA



Incarlopsa es una empresa familiar de capital 100% español. Desde 1978, su objetivo es producir y elaborar productos cárnicos porcinos de calidad.



Contamos con un modelo de producción vertical que garantiza la trazabilidad total del proceso productivo y la máxima calidad de nuestros productos.

La calidad, la seguridad alimentaria y el respeto al medioambiente articulan nuestro modelo de negocio sostenible donde la innovación desempeña un papel fundamental.



Dr. Miguel Martínez AGROVIN



Dra. Ana Belén Cifuentes

Liderazgo inspirador: Palanca clave para la innovación



La Dra. Ana Belén Cifuentes tiene la Licenciatura en Ingeniería Química por la Facultad Ciencias Químicas UCLM (Ciudad Real). Ha realizado varios Master, Máster integrado Seguridad, Medioambiente y Calidad (2004), Máster Superior de Gestión de Mantenimiento (ISE) (2006). Ha participado en varios programas de formación, Programas Management y Liderazgo (ESADE) (2015-2022) y de formación específica sobre procesos industriales: Destilación práctica (Kister), Procesos catalíticos fluidos (Exxon), Procesos extractivos Merox (UOP), Coquización retardada.

Desde la finalización de los estudios, toda su experiencia laboral la ha desarrollado en el Complejo industrial de Repsol en Puertollano. Entre 2004-2021 en el área de Producción de Refino y desde 2021 en HSE del Complejo integrado Refino-Química:

- 2004-2008 Jefe de Fábrica Refino
- 2008-2013 Jefe de Planta Unidad de Cracking Catalítico Fluido (FCC) (Repsol)
- 2013-2015 Técnico de unidades de Coquización y Destilación a Vacío (Repsol)
- 2015-2017 Técnico de Personal/Formación Conversión (Repsol).
- 2017-2021 Gerente de Movimientos y Entrega de Productos (Repsol)
- 2021-Act. Subdirectora de Seguridad, Medioambiente y Calidad del Complejo Industrial Repsol

Además, los proyectos transversales más destacados implantados en la Compañía:

- 2015-2021 Coordinadora de la implantación de Simuladores de Proceso Genéricos (OTS) como herramienta de entrenamiento del Operador de Panel en Complejos industriales de Repsol.
- 2020-2022 Agente del cambio en proyectos digitales sobre Nuevas formas de trabajo, Herramientas digitales para descarga de productos y herramientas de gestión HSE.

Elena Briñas

A new methodology for the quantification of graphene oxide in water sample



The use of graphene oxide (GO) increases in many products due to its vast number of excellent properties [1]. However, this extensive use in real-world applications has increased their potential release into the environment. In order to evaluate their possible health and ecological risks, there is a need for analytical methods that can quantify these materials at very low concentrations in environmental media such as water. One of the most sensitive analytical techniques is Raman spectroscopy (Fig. 1), specifically its most innovative variant, surface-enhanced Raman scattering (SERS) [2]. SERS is a good alternative for detecting GO with high selectivity and sensitivity. Indeed, given its potential for extremely high enhancement levels, SERS transforms Raman spectroscopy from a structural analytical tool to a structurally sensitive single-molecule probe [3].

Therefore, a new method for detecting and quantifying GO in aqueous samples is showed in this work [4]. The final methodology has been optimized and has shown is simple, useful, and effective in water samples. This method is able to detect GO in the concentration range of 0.1–10.0 ppb (Figure 1). The practical limit of quantification achieved is 0.1 ppb. This method shows high reproducibility and repeatability. Tests have been applied to real samples, showing good selectivity. And finally, in the case of accuracy, the recoveries obtained ranged from 95.66% to 100.47%.

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Almudena del Campo

PI3K inhibition using nanoparticles conjugated with the anti EGFR antibody Cetuximab for the treatment of Head and Neck Squamous Cell Carcinoma

Even though surgery approaches, radiation therapy and the use of therapeutic agents, the prognosis of head and neck squamous cell carcinomas (HNSCC) remains poor with tendency to develop recurrence and/or metastasis. In this regard, Inhibition of PI3K α is a promising therapeutic approach for the treatment of this tumor type¹. Epidermal growth factor receptor (EGFR) is overexpressed in over 90% of head and neck tumors² and, therefore, targeted therapies based on the antibody targeting EGFR is an alternative to be pursued. In this study, by the generation of anti-EGFR conjugated nanoparticles (ACNPs) for the controlled release of Alpelisib, a PI3K α inhibitor in clinical use, we propose a more efficient therapy for the treatment of HNSCC. Our study shows that the use of ACNPs aim to improve therapeutic efficacy by increasing the tumor concentration of Alpelisib which may reduce drug exposure in disease-free organs. The Alpelisib-loaded nanoparticles generated significantly enhanced efficacy *in vitro* in comparison with the free drug. These results proposed a novel strategy based on nanotechnology to enhance the efficacy of Alpelisib and diminish toxicity in patients with HNSCC.

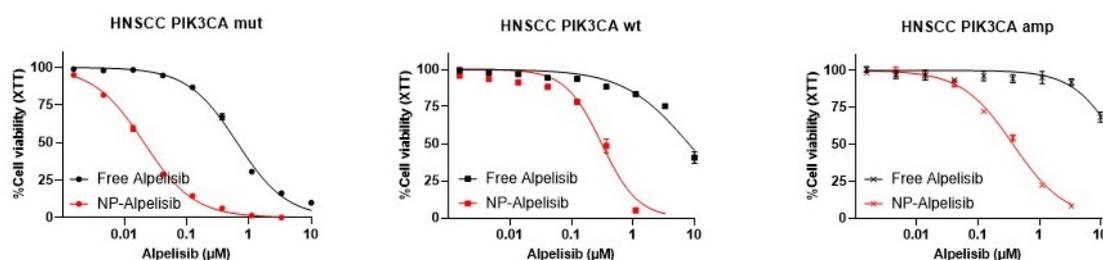


Figure 1. Antiproliferative effects induced by free Alpelisib and Alpelisib encapsulated in nanoparticles in three different cell lines at 72 hours

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M^a Pilar Castro

Persulfates electrogeneration using BDD anodes and 3D-printed reactors



Nowadays, one of the most important environmental problems is the pollution of liquid effluents due to the wide variety of refractory species that biological processes cannot treat. In this sense, the generation of oxidant species with high stability and high activity in the degradation of persistent pollutants emerges as an interesting alternative to traditional processes. Among the different technologies, electrooxidation with conductive diamond electrodes is one of the most efficient processes in the generation of oxidants due to the use of these diamond anodes favors the massive generation of strong reactive oxygen species, mostly hydroxyl radicals (HO^\bullet), at the surface of the anode [1]. The HO^\bullet produced react with other ions contained in wastewater favoring the production of other powerful oxidants. Among them, persulfates, widely used in many applications, are generated in presence of sulfate ions. Moreover, boron-doped diamond (BDD) anodes present higher chemical and electrochemical stability than other electrode materials, making them a good choice for persulfate generation [2]. Nevertheless, for its large-scale application, there are still many aspects to improve, some of which are addressed in this work. Therefore, this work is focused on the persulfate electrogeneration using BDD anodes with a novel 3D printing designed electrochemical reactor, paying attention to the influence of the key operation parameters (temperature, pH, current density, and electrolyte concentration) to determine the best conditions to produce persulfates efficiently and eco-friendly. This will not only contribute to the optimization of the persulfate generation process but also relevant economic savings in terms of materials and operational time can be achieved. Results show that the conductive diamond electrolysis of 1M of H_2SO_4 generates up to 0.2 M of persulfate with an anodic efficiency of 80%, being current density a key operation parameter with an optimal value of 300 mAcm^{-2} .

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M^a Arenas-Moreira

Enhanced antitumoral activity when combining PARP inhibitors with encapsulated BET inhibitors for the treatment of BRCA-mutated cancers

BRCA1/2 protein deficient or mutated cancers comprise a group of aggressive malignancies. Although PARPis have shown great efficacy in their treatment, the widespread use of these agents in clinic is restricted by various factors, including the development of acquired resistance due to the presence of compensatory pathways [1]. BETis can disrupt the HR pathway completely by repressing the expression of BRCA1 and could aim at generation combination regimes to overcome PARPis resistance and enhance PARPis efficacy [2].

Due to the poor pharmacokinetic profile and short half-life [3], the first in class BETi, JQ1, were loaded into newly developed nanocarrier formulations to improve the effectivity of Olaparib for the treatment of BRCA-mutated cancers. First, polylactide polymeric nanoparticles were generated by double emulsion. Also, liposomes were prepared by injection and evaporation solvent method. JQ1-loaded drug delivery systems display optimal hydrodynamic radii between 60 and 140 nm with a very low polydispersity index (Pdl), and encapsulation efficiencies of 98 and 45% for lipid- and polymeric-based formulations, respectively. Formulations show high stability and sustained release. We confirmed that all assayed JQ1 formulations display improved anti-proliferative activity compared to the free JQ1 in models of ovarian and breast cancers. In addition, synergistic interaction between JQ1 and JQ1-loaded nanocarriers and Olaparib evidenced the ability of encapsulated JQ1 to enhance antitumoral activity of BETis. In vivo studies validate the encapsulation of JQ1 as an efficient approach to combination therapies for the treatment of BRCA-mutated cancers.

Overall, these novel formulations may represent an efficient and safer JQ1-delivering alternative to enhance efficacy of Olaparib for BRCA-mutated cancer treatment.

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Inés M. Ramos Monge

Improvement of the texture of non-fat yogurt with autochthonous exopolysaccharides-producing LAB strains



Fermented foods have been consumed over the years and during this time they have been modified and improved according to trends and scientific advances. For some time now, consumers have been demanding more healthy and safe foods with as few additives as possible. Among these fermented foods is yogurt, which is consumed by the population almost every day. In the search for healthier foods, non-fat yoghurts were elaborated, which provide the nutrients of a traditional yogurt with less fat. However, the production of this product requires the use of thickeners to obtain the texture characteristics of a full fat yogurt. In the search to improve the texture of non-fat yogurts, exopolysaccharides (EPS) have begun to be used, which are carbohydrate polymers capable of producing thickening or gelling, providing products with pleasant rheological and sensory properties. These compounds are synthesised by microorganisms such as *Leuconostoc* and *Lactobacillus*, which are genera of lactic acid bacteria used in food processing.

In this work, experimental non-fat yogurts were produced with the addition of previously selected autochthonous EPS-producing LAB strains. Two strains of *Leuconostoc* (Ln2 and Ln6) and one of *Lactobacillus* (Lb47) were used to obtain non-fat yoghurts with the texture and organoleptic characteristics of this product, without the addition of thickeners or gelling agents as additives. The experimental yogurts were analysed physico-chemically, microbiologically and sensorially during a storage period of 28 days at 4°C. EPS production by the inoculated bacteria was found in all of them. Experimental yogurts were obtained with the characteristics of non-fat yogurts and no defects were found in any of them.

Manuel Bartolomé

Novel and sensitive electrochemical approach based on an assembly nanocomposite with chitosan and cyclodextrin-graphene quantum dots modified SPCEs for the full sensing of fluoroquinolones in alimentary samples



Fluoroquinolone (FQs) antibiotics have been used in an abusive way within the alimentary industry in the last decades, leading to the appearance of quinolone resistant microorganisms and reducing so the effectiveness of FQs-based drugs for the treatment of infection diseases at both animal and human levels¹. In consequence, diverse international organizations have established legislation regarding the maximum amount of quinolones allowed in food². A new electrochemical platform based on screen printed carbon electrodes (SPCE), modified with a nanocomposite material assembled from gamma cyclodextrins functionalized graphene quantum dots and chitosan (δ CDs-GQDs-CHI), has been reported and applied for the first time to evaluate the global amount of fluoroquinolones in food samples from animal origin. Electrochemical properties of the sensing nanocomposite were assessed by cyclic voltammetry (CV), showing improved electrocatalytic performance throughout evaluation of relevant electrochemical features as electronic transfer rate (K^0), electroactive area (A) and double capacitance layer (Cdl). Electrochemical mechanism of the redox process was also studied on four representative quinolones attending to their distinctive chemical structures, obtaining in all cases the same number of e^- (2) and H^+ (2) involved in their oxidation process, which suggested a single oxidation mechanism for all FQs, also here elucidated. Developed sensor shows boosted analytical performance in terms of linear range (4 – 250 μ M) and lower detection limit (LOD = 1.2 μ M). The designed approach allowed the determination of FQs global contain in broths, bouillon cubes and milkshakes at three concentration levels (150, 75 and 37.5 μ M) for both equimolar and different ratio FQs mixtures with recoveries values ranging from 90 to 106%.

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Carmen Soriano Herrador

Role of PPAR β/δ in the hypothalamic action of leptin. Implication on the inflammatory response and the control of food intake and energy expenditure



Leptin is an adipokine that acts at the hypothalamic and media level in the maintenance of energy homeostasis and the control of intake. PPAR β/δ is a transcription factor involved in lipid metabolism and the inflammatory response. The relationship between leptin and PPAR β/δ in different peripheral tissues is known, however, at the hypothalamic level it has not been fully clarified. The main objective of this work was to study the role of PPAR β/δ in the action of leptin in the hypothalamus and its relationship with the modulation of the inflammatory response and the production of neuropeptides involved in the control of energy intake and metabolism.

GSK0660, a PPAR β/δ antagonist, was used and administered intraperitoneally (IP) for 7 days to 3-month-old Wistar rats, which were simultaneously administered leptin or saline intracerebroventricularly via osmotic minipumps. On the hypothalamic tissue, the expression levels of PPAR β/δ were analysed together with their targets. Thus, it was observed that the combined administration of leptin and GSK0660 produced a decrease in the levels of these factors, demonstrating that the PPAR antagonist was able to cross the blood-brain barrier. The effect that PPAR β/δ had on the leptin pathway was studied. The transcription factor increased the pathway activation by increasing levels for the adipokine receptors and for SOCS3 and pY727-STAT3. In addition, the involvement of PPAR β/δ in the neuroendocrine activity of leptin was determined. The results obtained showed that GSK0660 caused an increase in the secretion of orexigenic factors (NPY) and a decrease in the anorectic ones (POMC, TRH, CRH), contrary to the effect of leptin. Finally, the involvement of PPAR β/δ in the hypothalamic inflammatory response was determined. Blocking this factor increased the levels of pro-inflammatory factors (CCL5) and microglial and/or macrophages and astrocytes markers (Iba1 and GFAP, respectively). On balance, the values obtained seem to show that PPAR β/δ is involved in the hypothalamic functions of leptin and that it would have an anti-inflammatory effect at this level.

Sergio Pozuelo-Campos

Strategies for Robust Designs in Toxicological Tests



Toxicological tests are widely used to study toxicity in aquatic environments. Reproduction is a possible endpoint of this type of experiment, whose response variable is given by counts. There is a literature on the most suitable probability distribution to be used for analyzing the data. In the theory of optimal experimental design, the assumption of this probability distribution is essential, and when this assumption is not appropriate, there may be a loss of efficiency in the design obtained. The main objective of this study is to propose robust designs when there is uncertainty about the probability distribution of the response variable. Three different strategies for attaining this goal are introduced and compared, and they are then applied to toxicological tests based on and *Lemna minor*. In addition, a simulation study is performed to test the estimation properties of the robust designs obtained.

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María Areti I. Spanoudaki

Atmospheric chemistry of Hydrochlorofluoroolefins(HCFO): Why is it important?



Halogenated unsaturated olefins, i. e., Hydrofluoroolefins (HFO) have been recently proposed as Hydrofluorocarbons (HFC) replacements. Although CFC and HCFC are controlled by the Montreal protocol and its amendments, the high atmospheric reactivity of the double bonds in Hydrochlorofluoroolefins (HCFO) towards atmospheric oxidants like OH radicals or Cl atoms prohibits them from being transferred in the stratosphere leading to short tropospheric lifetimes, very low GWPs¹ and negligible ODPs. Further, the presence of the C-Cl bonds along with the C-F enhances the required physicochemical properties of HCFO,² extending the field of their potent applications. As of today, $\text{CF}_3\text{CF}=\text{ClCH}$ and $\text{CF}_3\text{CH}=\text{ClCH}$ are already used as refrigerants and blowing agents.^{3, 4} However, HCFO are not included in the Paris Agreement and they are not regulated by the Kigali Amendment of the Montreal Protocol, while at the same time, there are very limited data regarding their atmospheric reactivity and almost none about their oxidation end-products. Prior to their extensive production and use, the full atmospheric lifecycle of HCFO needs to be assessed so as to evaluate their impact on climate change and air quality. In this study the reaction kinetics of OH radicals with $\text{CF}_3(\text{Cl})\text{C}=\text{CCl}_2$, at atmospherically relevant temperatures will be investigated in the department of Physical Chemistry of UCLM, employing the Pulsed Laser Photolysis/Laser Induced Fluorescence (PLP/LIF) technique⁵ and a smog simulation chamber⁶.

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Pablo Belmonte López

Study of Process Variables on the Microcellular Foaming of Different TPUS using Supercritical CO₂



Polyurethanes (PU) are part of the “big six”, a group gathering the six most important plastic materials worldwide for their use and economic value. The main problem derivate from the extensive use of these materials is the high number of wastes related to their synthesis and what to do with these materials after their lifetime. For this reason, the present work proposes as an alternative to the traditional recycling of thermoplastic polyurethane the foaming of this material using supercritical CO₂.

The present work is focused on the study of the influence and significance of temperature, pressure, and contact time with the supercritical CO₂ in the foaming of thermoplastic polyurethanes (TPU). To carry out the study of these variables, four commercial TPUs were selected.

The following range of conditions were studied, using a design of experiments and an statistical software to analyze the data (Statgraphics):

- Temperature: 100 °C – 120 °C
- Pressure: 100 bar – 200 bar
- Contact time: 1 h – 3 h

TPUs were characterized using DSC and TGA analysis to determine the melting point and the thermal degradation temperature of the polymer. Once foaming experiments were done, the density of the foams obtained was measured using a 3D scanner SEM analysis were also performed with the aim of analyzing the foam structure obtained. Using the information provided by the density measurement and SEM, cell density (Nf), average cell size (D), and expansion ratio (Φ) were calculated for the different conditions studied.

Carlos Martín

Bilayer hydrogel in drug delivery



Tissue engineering is an interdisciplinary field in continuous development, combining progress in technology and life sciences. This area has great potential in regenerative medicine, and its greatest achievement could be to generate artificial organs from cells, supports and biological factors. Among the different materials that can be used in tissue engineering, hydrogels represent a class of macromolecules of particular interest because they possess unique physicochemical characteristics, which make them the synthetic biomaterials that most closely resemble living tissues.[1] Hydrogels prepared from natural polymers do not have good mechanical properties, although they have the advantage of being biocompatible and biodegradable. On the other hand, synthetic hydrogels can be synthesized with greater control of their mechanical properties: their highly porous structure can be easily tailored by controlling the crosslink density and the type of functional groups in the gel matrix. However, they are not as biocompatible as natural hydrogels, and their biodegradation is difficult and/or they can produce toxic degradation compounds. In this work, in order to combine the advantages of synthetic and natural hydrogels, a bilayer hydrogel is prepared: a smart synthetic hydrogel layer that will respond to external stimuli attached to a natural hydrogel layer, where the cell culture will be performed (Figure 1). The swelling degree of both gels, their internal structure using the scanning electron microscopy technique and their mechanical properties (Young's modulus and viscoelasticity) have been analyzed. In addition, the release of rhodamine 101 from these gels has been studied in response to a magnetic stimulus.

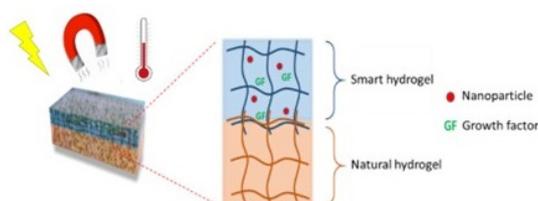


Figure 1: Bilayer hydrogel

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Raquel Muñoz

Behaviour of Oenological Microorganism after Microwave Treatments



Microwave has been more frequently used in food industries to enhance or replace conventional techniques. The present study will focus on the application of microwaves (MW) on microorganisms to evaluate its effect with different treatment conditions of power, duration and presence of pulses on *Saccharomyces* and *non-Saccharomyces yeasts* and *Lactiplantibacillus plantarum*; studies of viability and vitality were carried out after treatments. MW affected all microorganisms in different ways depending on the applied treatment and on the microorganism. In general, *S. cerevisiae* and non-*Saccharomyces* yeast were less resistant than *L. plantarum*. Counts immediately after treatment showed influence reaching even inactivation. Nevertheless, maximum OD after 96 h presented values closer to the controls (microorganisms not treated). This effect shows that in some cases the treatment exerts an antimicrobial effect immediately after application, but after some time, microorganisms can restore their biological structures and growth, which is reflected in an increase of lag phase. On a few occasions, treatments were also able to improve the kinetic parameters. Thus, this technique could be useful for inactivation, attenuation, or even activation of associated food microorganisms.

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Marina Pinzón

Novel Carbon-Based Catalysts for Hydrogen Production from Ammonia Decomposition



1. Introduction

Currently the success of the 'hydrogen economy' depends on the current hydrogen (H_2) storage and transport routes, which are characterized by their high costs (high pressures or low temperatures)¹. A potential solution to this issue comprises the utilization of molecules that contains hydrogen in its structure such as ammonia (NH_3). Because of high hydrogen content, mature technology and relatively low cost (easy liquefaction), and carbon-free molecule, ammonia has gained attention as 'hydrogen carrier' to generate H_2 . Unfortunately, H_2 from NH_3 requires an efficient catalyst to achieve high conversion at low reaction temperatures. Recently, attractive results have been obtained with carbon-based materials due to their high electron conductivity, adequate basicity, surface area, thermal stability as well as the absence of electron-withdrawing species². Moreover, ruthenium (Ru) active sites are improved over carbon materials as consequences of the small size of Ru and high dispersion³⁻⁵. Indeed, ammonia decomposition is a structure-sensitive reaction, particles in small size enhance this reaction⁶. Ru supported on graphene have been studied for this reaction, but these materials implied high Ru amount (>10 wt%), and complicated synthesis method⁵. In this context, Ru supported on reduced graphene oxide (rGO) were synthesized, characterized and tested for carbon-free H_2 generation from NH_3 , for the first time. Ru loading as well as the incorporation of different amounts of pre-reducing agent (2-chloroethylamine hydrochloride) were optimized.

2. Experimental Section

The supports (yC-rGO) were prepared by mixing graphite oxide (40 g·L⁻¹) with the pre-reducing agent amount (y=0, 10, 20 and 40 g). The mixture was sonicated for 4 h and transferred into a Teflon-lined autoclave for hydrothermal treatment (180 °C for 12 h). Then, the product was filtered under vacuum and calcined at 500 °C (3 h) and 200 °C (2 h) in nitrogen. Finally, it was centrifuged, washed several times to neutral pH and dried by lyophilization. The metal incorporation of the active metal phase (Ru) was carried out through a modified hydrothermal method over 20C-rGO. For this purpose, the desired amount of $RuCl_3 \cdot 3H_2O$ was added over 2 g·L⁻¹, sonicated for 1 h, and reduced with hydrazine in a 1:1 weight ratio with respect to the support. The mixture was transferred to an autoclave reactor (180 °C for 12 h), centrifuged, washed several times to neutral pH and dried (xRu/20C-rGO, where x= 1, 2.5 and 5 wt% of Ru).

The catalysts were characterized by elemental analysis, SEM, XRD, HRTEM, H₂-TPR and CO₂-TPD. Catalytic tests were performed in a fixed-bed reactor using 0.04 g of samples and a flow rate of 100 ml·min⁻¹ with 5% NH₃/Ar (v/v). The products were analysed by chromatography. Finally, the stability of selected catalysts was tested at 400 °C for 65 h.

3. Results and Discussion

The catalytic activity of the γRu/20C-rGO catalysts (Table 1) previously treated in situ at 200 °C with 10% H₂/Ar, increased with the reaction temperature as a result of an improvement in the reaction kinetics. In the absence of active phase, NH₃ conversion only achieved 4% at 400 °C. Note that, ammonia conversion increased with the Ru load because of an increase of the amount of active sites. However, 5Ru/20C-rGO catalyst showed a particles size of 8.8 nm, which did not improve the B5 type-sites (Figure 1)⁶. Thus, 2.5Ru/20C-rGO exhibited a Ru size of 3.6 nm presenting the optimal one to achieve a 91.2% of ammonia conversion. For that reason, this Ru loading was selected as the optimal to carry out the following experiments.

Table 1 – NH₃ conversion of samples at 400 °C.

| Samples | Ammonia conversion (%) |
|---------------|------------------------|
| 20C-rGO | 2.5 |
| 2.5Ru/20C-rGO | 91.2 |
| 1Ru/20C-rGO | 52.2 |
| 5Ru/20C-rGO | 95.3 |
| 2.5Ru/0C-rGO | 63.5 |
| 2.5Ru/10C-rGO | 96.3 |
| 2.5Ru/40C-rGO | 90.4 |

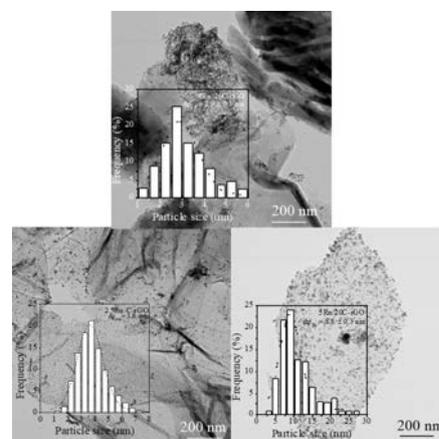


Figure 1 – TEM images of xRu/20C-rGO catalysts

As observed, a clear increase in the ammonia conversion took place when pre-reduction was carried out (Table 1). In fact, 2.5Ru/10C-rGO showed the highest ammonia conversion, which was associated with highly crystalline structure with few structural defects, adequate surface area and the highest basicity (1.69 mmol CO₂ gcat⁻¹). The low catalytic performance obtained with 2.5Ru/0C-rGO catalyst was due to its poor structural order (low crystalline character) being the effect of N-functionalities masked by this high structural disorder. In this sense, higher elimination of oxygen functional groups, graphitic structure and high basicity are key factors to develop an efficient Ru supported on reduced graphene oxide catalyst. Additionally, 2.5Ru/10C-rGO showed the highest ammonia conversion at the lowest temperature with the lowest Ru amount of catalysts available in the literature⁴, presenting an ammonia conversion of 96 % at 400 °C for more than 65 h of reaction.

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Josué Muñoz Galindo

Sulfonate-based Hydrogels: New Soft Scaffolds for Biomedical Applications



The concept of tissue engineering has been widely studied. It involves from the field of biomaterials to scaffolds for cell culture. The final goal is to design materials which will be able to mimic human organs or tissues that can replace or repair damaged or diseased tissues with scaffolds made through the combination of natural and synthetic components.¹

In that sense, hydrogels have recently attracted much attention in the field of tissue engineering, having numerous applications, especially as scaffolds for cell cultures.² We have shown that the introduction of graphene in the hydrogel structure improves their biocompatibility supporting the growth of cultured brain cells and allowing neuronal adhesion.³

In this work, novel graphene hybrid hydrogels based on sodium 4-vinylbenzenesulfonate (VBS) have been prepared in order to study their capacity to support living neurons.

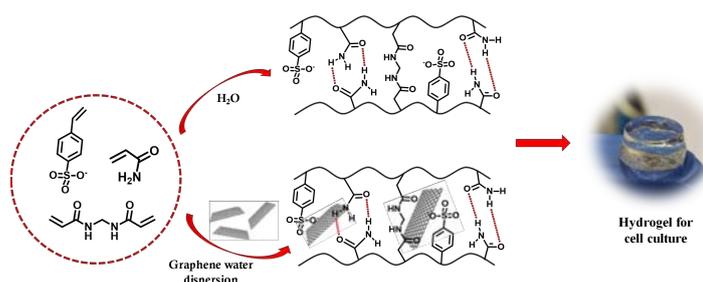


Figure 1. VBS based hydrogels in the presence and absence of graphene.

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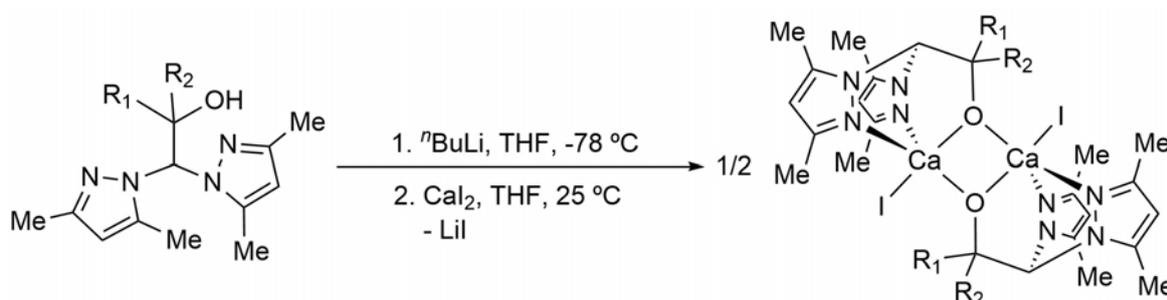
Enrique Francés-Poveda

Calcium complexes as catalysts for activation of small molecules



In recent years, great advances have been made in the design of catalysts based on abundant and/or biocompatible metals for their use in the transformation of CO₂ into high value-added products. For instance, metals such as aluminium, iron, or zinc, have shown to be efficient catalysts for the synthesis of new organic molecules and polymeric materials with CO₂ in their structure [1]. In this sense, calcium is a metal that could also be especially useful in this type of catalytic process, considering its abundance, easy availability, and low cost. In addition, it is a biocompatible metal, so its use in processes that involve obtaining materials with subsequent applications in biomedicine is of great interest.

Despite all of this, there are hardly any studies to date on the use of calcium catalysts in CO₂ activation processes, so it is highly relevant to delve into the use of these metal complexes for this type of development [2]. In this context, new calcium complexes supported by heteroscorpionate ligands have been prepared by reaction of Ca₂ with the lithium salt of different bis(3,5-dimethylpyrazol-1-yl)methane-based ligands (Scheme 1). The reactivity of these complexes towards CO₂ and other small molecules has also been evaluated. Furthermore, these calcium compounds have been used as one-component catalysts for the synthesis of cyclic carbonates from epoxides and propargyl alcohols and CO₂ under mild reaction conditions.



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Natalia Villamayor

Fluorescent discrimination between free and nanoencapsulated quercetin by a quenching responsive nanotool based on S,N-graphene quantum dots



A new smart nanomaterial based on sulfur and nitrogen co-doped graphene quantum dots (S,N-GQDs) has been synthesized for both detection and discrimination of free and encapsulated quercetin as nanoemulsions-loaded (Q and Q-Nes respectively). The sensing nanoprobe was reached by a hydrothermal single step through a bottom-up approach [1]. The presence of Q-NEs and free Q can quench the S,N-GQDs fluorescent intensity through an inner filter effect (IFE) mechanism exhibiting a dynamic quenching for Q-NEs and static one for free Q (Figure 1). A low energy method, such as phase inversion temperature method (PIT) was selected to synthesize Q-NEs [2]. The optimal Q-NEs composition (% w/w) was: 10% Miglyol 812, 0.25 % quercetin, 0.55 % ethanol, 7.4 % tween 80, 0.1 % soy lecithin and to 100 % of aqueous phase (MES buffer pH = 5.9). All synthesized nanomaterials were characterized through DLS, CLSM, SEM, HRTEM, XRD, FTIR, Raman, UV-Vis and fluorescence spectroscopies in order to describe their physic-chemical and nanostructural features.

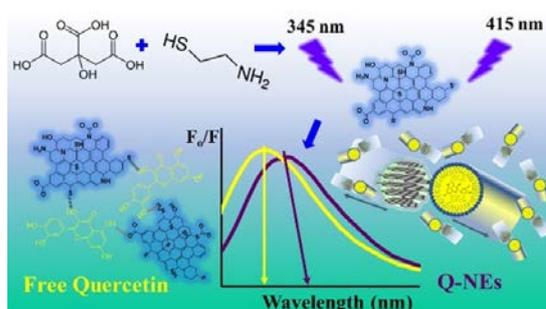


Figure 1. Discrimination between Q and Q-NEs through their quenching behaviour.

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Adrián Tejero Pérez

Effect of glutamate intake during gestation on the cerebellum of pregnant rats and their fetuses: an overview of the state of receptors and oxidative stress



Glutamate is an amino acid present in proteins that we usually ingest in the diet, but its consumption has increased significantly since it is an important additive, responsible for the umami flavour, that enhances the flavour of foods. This amino acid is needed to synthesize endogenous proteins, but it also plays a fundamental role in the central nervous system (CNS), being the main excitatory neurotransmitter. At physiological concentrations, it participates in learning and memory processes, however, at high concentrations it acts as an excitotoxin producing cell degeneration and death. In fact, high concentrations of this amino acid have been associated with neurodegenerative diseases (ND). Glutamate and adenosine (which modulates glutamate level) receptors have been studied in different ND resulting in a significant alteration of its expression or affinity in different tissues. Not only that, but the study of the oxidative stress correlated with ND such as Alzheimer disease (AD) and Parkinson disease (PD) is key to understand the etiology of these diseases and to reach new strategies of early diagnosis and treatment. Previous studies of this group have shown that there is a change in the receptor expression in the brain of pregnant rats administered glutamate and their fetuses but is unknown what happens in the cerebellum of these animals. Cerebellum is abundant in neurons and it is responsible for motor, cognitive and emotional functions, and this structure can also be useful in the study of AD and PD. Therefore, the aim of this research is not only to analyze the receptors expression in the cerebellum, but also focus on the study of the oxidative stress associated to the consumption of glutamate. The state of the receptors seems to remain unaltered in cerebellum, unlike in brain, however the oxidative damage caused by glutamate consumption is significant as it is seen in enzymatic activities and peroxidation assays carried out on this samples. Further studies will be necessary to elucidate the importance of glutamate intake and its possible excitotoxicity in cerebellum of pregnant rats and their ability to cross the placental barrier.

The catalytic co-fast pyrolysis of OP mixed with PVC was performed in a Py-GC/MS (CDS Pyroprobe 6200 pyrolyser and Agilent Technologies 7890B/5977B GC/MS). Different experiments were performed using a biomass to PVC ratio previously optimized (1:1.5 OP/PVC) adding zeolite catalyst varying total mass proportions (2:1, 1:1 and 1:2). Fast pyrolysis reaction was employed at 650 °C with a heating rate of 20 °C/ms and a residence time of 20 s. These operational conditions and the selected OP/PVC ratio were optimized and selected in a previous study [4].

3. Results and Discussion

The product yield from the pyrolysis of biomass/zeolite, as well as raw materials are shown in Figure 1. The components detected in the bio-oil were divided into two groups: hydrocarbons and oxygenates. Hydrocarbons were mainly composed of olefins, cyclic hydrocarbons and aromatics, which were divided into monocyclic aromatic hydrocarbons (MAHs) mainly benzene, toluene and xylene (BTX); and polycyclic aromatic hydrocarbons (PAHs). Moreover, oxygenates production was based on alcohols, aldehydes, carboxylic acids, esters, ketones and phenols. Fig. 1 A) shows that yields of hydrocarbons in the non-catalytic fast pyrolysis of OP peaked at 25%, while the remainder were oxygen-containing compounds. The most representative were phenolics (from thermal decomposition of lignin) and carboxylic acids (from the acidic nature of feed). When NaZSM-5 was added to the sample, hydrocarbon compounds fell, and oxygenated products rose. The total percentage of hydrocarbons reached to 28.3% for 1:2 OP-NaZ, which was made up of 16.5 and 11.8% of olefins and cyclic hydrocarbons, respectively. This might have been due to the combined catalytic action of AAEMs inherent in OP and the sodium contribution from NaZSM-5. In this case, the zeolite in the sample combined with the catalytic effect of the inherent AAEMs (especially K, 3.48 wt.% (Table 1)) led to a fall in oxygenates at the expense of a slight rise in the formation of hydrocarbons. When HZSM-5 was used as a catalyst, oxygen content dropped whereas aromatics rose in comparison with the raw biomass. With a greater ratio of zeolite in the mixture, hydrocarbon production was enhanced, which peaked at 95 % in 1:2 OP-HZ. The yield of MAHs was higher than that of PAHs. However, BTX appeared in the bio-oil with toluene being the most prevalent. As a special polymer, PVC was selected to be studied in co-pyrolysis with biomass despite its low H/C_{eff} in comparison to other polyolefins. Compared to the non-catalytic fast co-pyrolysis of the OP/PVC blend, the presence of the HZSM-5 zeolite promoted the formation of aromatics while decreasing the amount of aliphatic hydrocarbons and oxygenate compounds (Fig. 1 B). Production of aromatics in OP/PVC experiments was high, and was slightly enhanced with HZSM-5, from 64 % in 1:15 OP/PVC to 70 % in 1:2 OP/PVC-HZ. In this case, BTX selectivity significantly increased, with toluene being the main aromatic detected. Thus, in 1:2 OP/PVC-HZ, a maximum yield of 19 % was obtained, higher than that in the raw materials OP (12 %) and PVC, which was not detected. Meanwhile, yields of PAHs fell, especially in 1:2 OP/PVC-HZ (in which selectivity for BTX was much higher than that for PAHs).

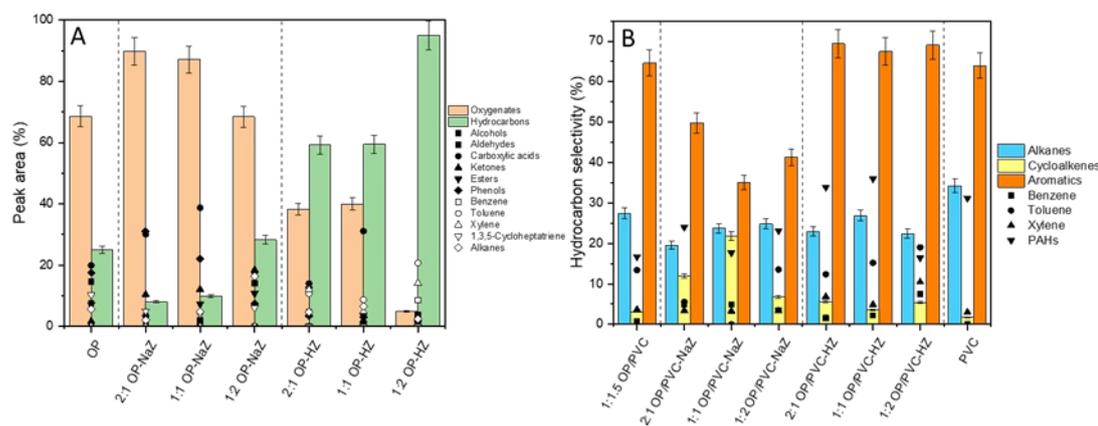


Figure 1. A) Product yield obtained from the catalytic fast pyrolysis of OP over NaZSM-5 (OP-NaZ) and HZSM-5 (OP-HZ) zeolites and B) Hydrocarbon selectivity obtained from catalytic fast co-pyrolysis of 1:1.5 OP/PVC over NaZSM-5 (OP/PVC-NaZ) and HZSM-5 (OP/PVC-HZ) zeolites

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Abelardo Sánchez-Oliva

Rational Design of D-A-D Naphthalenediimide and Perylenediimide with Potential Applications as n-Type Semiconductors in Organic Field-Effect Transistors



In the last decades, organic molecules have attracted the interest of the research due to their enormous potential in electronic devices like organic field-effect transistors (OFETs). In this way, an interesting strategy is to build donor-acceptor-donor (D-A-D) architectures, making easier intramolecular charge transfer (ICT), necessary for this kind of devices. In this sense, naphthalenediimide (NDI) and perylenediimide (PDI) derivatives are very interesting due to their planar structure, their acceptor character, their self-assembling capacity and the possibility of combining with different donor groups to obtain D-A-D systems. Furthermore, Computational Chemistry is a powerful tool in Organic Chemistry because it can predict properties of compounds before synthesizing them, avoiding unnecessary synthesis and contributing to more economic and sustainable processes. Taking into account all these premises, in this work, D-A-D naphthalenediimide and perylenediimide derivatives (Figure 1) with different alkynyl donor groups were chosen. Firstly, these compounds have been theoretically studied, then they were synthesized, and OFET devices were manufactured under different conditions. The results obtained from this study showed a behavior as n-type semiconductors with high electron mobilities, [1] improving the electrical efficiency with respect to previous D-A naphthalenediimide derivatives described by our research group. [2]

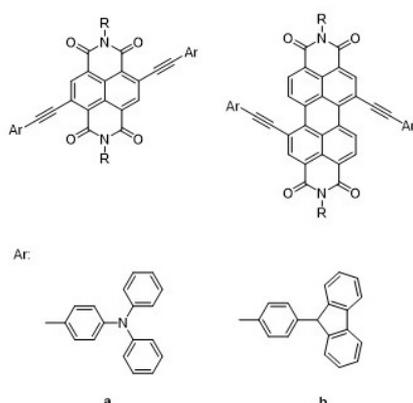


Figure 1. Different series of D-A-D naphthalenediimide and perylenediimide derivatives.

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Angel Alcázar-Ruiz

BTX Enhancement Production Through Catalytic co-fast Pyrolysis of Agricultural Waste



1. Introduction

Lignocellulosic biomass is an abundantly renewable feedstock for producing bio-oil with aromatic hydrocarbons via fast pyrolysis [1]. However, the bio-oil yielded has certain disadvantages in comparison to petroleum-derived oil: low calorific value, high viscosity, and thermal instability due to its composition of a mixture of oxygenated compounds. Moreover, the hydrogen-deficient nature of lignocellulosic biomass yields undesirable features in the bio-oil. Therefore, co-pyrolysis with hydrogen-rich material has become a simple way of enhancing both bio-oil quality and yields. To tackle the problems posed by bio-oil, plastic waste is presented herein as a solid feedstock for blending with biomass residue. Among the most used types of plastics, polyvinyl chloride (PVC) has attracted attention due to high consumption in recent years. Worldwide demand for PVC is expected to grow by 3.2% annually until 2023 [2]. To counter harmful emissions in PVC combustion by traditional plastic waste disposal techniques, enhanced recycling techniques that convert solid waste blends into high value-added products are urgently needed. To enhance the bio-oil obtained from co-pyrolysis, firstly, it must undergo catalytic upgrading using efficient catalysts to reduce its oxygen content and heavy hydrocarbons. Catalysts may be incorporated into co-pyrolysis, to remove oxygenated fractions via decarboxylation, dehydration and decarbonylation, to produce enhanced bio-oil. However, in combination with zeolites, some internal minerals in biomass, such as alkali and alkaline earth metals (AAEMs) could interact as catalysts and influence bio-oil yields and their composition [3]. This work addresses enhanced benzene, toluene and xylene (BTX) production by catalytic fast co-pyrolysis from agroindustrial biomass blended with PVC and the use of prepared NaZSM-5 and HZSM-5 zeolites. Moreover, the coupling effect of the AAEMs inherent to the biomass and zeolite on the production of aromatics was evaluated.

2. Experimental Section

Olive pomace (OP) was used as agricultural waste biomass feedstocks. It was supplied by Aceites García de la Cruz oil mill (Madrirdejos, Castilla-La Mancha, Spain). The used PVC was purchased from Sigma-Aldrich, US. Samples were characterized: ultimate and proximate analysis were carried out according to standards UNE 15104:2011, UNE-EN ISO18123:2016, UNE 32-004-84 and UNE 32-002-95; metal content was determined by Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES); and contents of extractives, hemicellulose and Klason lignin were determined according to TAPPI 204 om-97 and TAPPI T 222 om-02.

Maite Bernardo C. Dos Santos

Production of a Heterologous Ferulic Acid Decarboxylase Enzyme from *Klebsiella Pneumoniae* TD 4.7 and Application of the Enzyme in the Production of 4-Vinylguayacols



4-vinylguaiacol (4-VG), with a spicy clove aroma, is a valuable component in the food and cosmetics industry, particularly in the production of fragrances. However, the industrial demand for 4-VG is not met by extraction from natural sources and synthesis by chemical. As a solution, enzymatic methods can be used to produce these compounds. Bacteria are capable of transforming ferulic acid (FA) into 4-VG, where the bioconversion pathway occurs by the non-oxidative decarboxylation reaction by the action of the enzyme ferulic acid decarboxylase (FAD) (EC 4.1.1.102). The *K. pneumoniae* TD4.7 in the working collection at the Laboratory of Biochemistry and Applied Microbiology of São Paulo State University (UNESP-BRASIL), has an AFD gene. The FAD enzyme gene was amplified and the product was inserted into plasmid pET-28a(+). The pET-28a(+)/fad recombinant vector was transformed into *E. coli* BL21(DE3), and the induction of 0.2 mM IPTG at 20°C overnight, FAD was highly expressed as a soluble protein. Protein purification was performed and FAD enzyme activity was determined by assays carried out in triplicate, adding 0.05 mL of enzyme extract to 0.45 mL of a solution composed of 0.3 g L⁻¹ of FA. The reaction mixture was incubated at 40°C, at pH 5.5, for reaction times of 5, 10 and 15 min. FAD enzyme activity was measured by FA reduction and 4-VG formation. After the heterologous FAD purification process, SDS-PAGE polyacrylamide gel analysis was performed to verify the material, each isoform has a mass of approximately 20 kDa. The enzyme activity test showed that the enzyme maintained its activity after the cloning and heterologous expression processes in *E. coli*, confirming its catalytic efficiency for FA with 4-VG formation.

Angela Moratalla

Comparison of the Effect of Ozone and Chlorine Dioxide Dosing on Hospital Urine Polluted with Pharmaceuticals



1. Introduction

The inefficiency of conventional biological processes to remove pharmaceutical compounds (PhCs) is leading to their accumulation in aquatic environments. These compounds are characterized by high toxicity, high antibiotic activity and low biodegradability, and their presence is causing serious environmental risks [1]. Hospital effluents have been considered one of the main routes of entry of PhCs into the aquatic environment, as a large part of these compound are consumed by patients and excreted in the urine. In addition, it has been found that the concentration of PhCs in hospital effluents is approximately 25% higher than in municipal wastewater [2]. Therefore, it is important to develop efficient technologies to reduce the chemical and biological risk of this type of effluents. In this context, Electrochemical Advanced Oxidation Processes (EAOPs) have demonstrated high performance for degradation of organics compounds in wastewater thanks to the in-situ electrochemical generation of powerful oxidants in liquid and gas phase such as ozone (O_3) and chlorine dioxide (ClO_2). In this context, this work aims to test the feasibility of electrochemically generated O_3 gas and ClO_2 gas for application to hospital urine polluted with several PhCs of similar composition to the effluents of an Intensive Care Unit (ICU) ward.

2. Experimental Section

Firstly, a predictive model has been developed to visualize the occurrence of the most prevalent PhCs in hospital urine from the data provided by the Pharmacy Service of the University Hospital of Albacete, Spain (CHUA) related to the main PhCs provided in ICU wards. To do this, the total number of units of each compound supplied, the maximum urine excretion factor, the total number of bed and the daily flushed from the toiled per bed have been considered. The most prevalent PhCs present in urine from ICU wards were selected to prepare the synthetic urines and the degradation of polymedicated urines was evaluated with electrochemically generated O_3 and ClO_2 gas was evaluated. The experimental system used for gas-phase ozone treatment consists of an electrochemical system using a PEM (proton exchange membrane) cell and a gas phase ozone dosing system (Figure 1). The experimental set up used for gas phase ClO_2 treatment consists of a generation reactor where chlorate and hydrogen peroxide electrochemically generated were mixed to produce ClO_2 . In addition, an air pump is used to bubble air into the reaction mixture promoting the dragging of ClO_2 gas into the absorber (Figure 2).

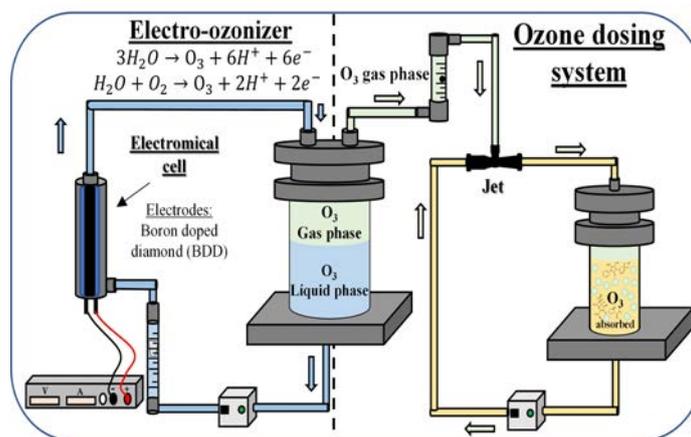


Figure 1. Ozone dosing system

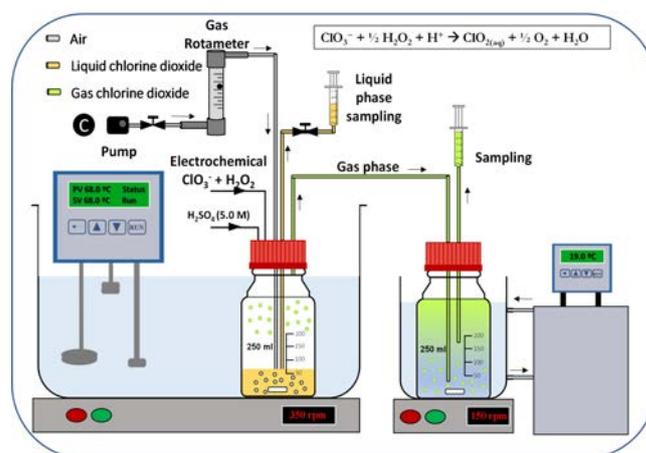


Figure 2. ClO₂ dosing system

3. Results and Discussion

Previous results showed that the most prevalent PhCs in hospital urine from ICU ward were antibiotics and analgesics and anti-inflammatories. Among the antibiotics, the maximum concentrations in hospital urine were highest for piperacillin and meropenem. For the analgesic and anti-inflammatory group, the most prevalent PhCs was metamizole. During the degradation of complex urines of hospital urines of ICU wards, O₃ and ClO₂ allowed the total removal of PhCs after treatment. However, lower kinetics constant and mineralization rates were observed in the case of ClO₂ treatment.

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Acknowledgments

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Clara Fructuoso González

Signal Transduction Pathways in a Tumoral Cell Line: What About Cholesterol Metabolism?



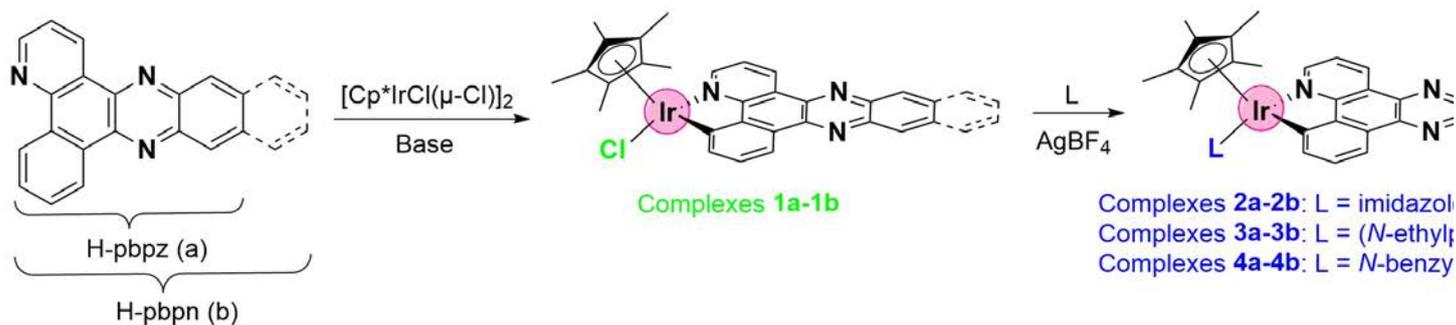
Transduction pathways are mediated by stimulation or inhibition of receptors, mainly G protein coupled receptors, in the plasma membrane by specific neurotransmitters. Glutamate is the main excitatory neurotransmitter in the Central Nervous System which is involved in physiological action as learning and memory processes. Action of glutamate is evoked by two types of receptors, ionotropic that are ion channel and metabotropic glutamate receptors which has been classified into Group I, II and III. Group I receptors are coupled to stimulation of phospholipase C activity and Groups II and III receptors are coupled to inhibition of adenylyl cyclase activity. At high concentration, glutamate is excitotoxic being responsible for degeneration and neuronal death. To avoid cytotoxic action of glutamate several neuromodulator molecules, such as adenosine, regulate levels of this neurotransmitter. Adenosine is a nucleoside that exert their neuroprotective role through four specific receptor, namely A1, A2A, A2B and A3 receptors. A1 and A3 receptor inhibit adenylyl cyclase activity while A2A and A2B receptors stimulate this enzymatic activity. Both adenosine and glutamate receptor have been involved in neurodegenerative diseases as Alzheimer Disease (AD). Recently, our group have described that cholesterol present in plasma membranes is able to bind and modulate adenosine receptors acting as a non-selective agonist suggesting that cholesterol in brain could be involved in the neurodegeneration characteristic of AD. Therefore, we try to elucidate the role of the metabolism of this lipid and their relationship with adenosine and glutamate receptors in degeneration and cell death using C6 glioma cell as a model. Lipoprotein, enzymes related to the cholesterol metabolism and transduction pathways have been analyzed. Preliminary results show an important relationship between lipid metabolism and signal transduction pathways mediated by adenosine and metabotropic glutamate receptors, mainly by modulation of cAMP levels. Additional studies will be necessary to suggest that the maintaining of cholesterol level not only is important to prevent cardiovascular but neurodegenerative disease.

Carlos Gonzalo-Navarro

Potential of sunlight in the treatment of diseases: photodynamic therapy at ultra-low doses to treat cancer



Photodynamic therapy (PDT) is a clinically approved non-invasive technique to treat cancer. In this strategy, a photosensitizer (PS) is delivered which is ideally harmless in the dark and activates in the presence of light releasing $^1\text{O}_2$ and reactive oxygen species (ROS), which can cause cell death. Octahedral Ir(III) complexes with C^N ligands have been employed as PS in PDT due to their photochemical properties.[1] In this work, new half-sandwich Ir(III) complexes with π -extended C^N ligands and imidazole derivatives (Fig. 1) are presented as PDT agents at ultra-low doses.



Biological studies in A549 cell line show high cytotoxicity in the dark for all complexes ($\text{IC}_{50} \leq 8 \mu\text{M}$). Under blue light, cytotoxicity hardly improves for pbpz but significantly increases for pbpn complexes ($\text{PI} = \text{IC}_{50,\text{dark}}/\text{IC}_{50,\text{light}} \leq 1300$) by a great $^1\text{O}_2$ generation ($\Delta \geq 0.81$), achieving $\text{IC}_{50,\text{light}}$ values up to 190 pM for 4b. Complexes with pbpn are activated even with red light ($\text{PI} \leq 63$), which allows a greater light penetration. These outstanding results confirm the enormous potential of pbpn complexes as $^1\text{O}_2$ sensitizers and as a new class of photoactivatable anticancer drugs.

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Fco. Javier Patiño

Potential of sunlight in the treatment of diseases: photodynamic therapy at ultra-low doses to treat cancer



It is beyond doubt that robotics plays an important role in our society, and that this area will be an important part of our future. However, at this moment most of the robots are only used in industry because they are made of hard materials such as metals, which can cause problems when treating with living beings.

In order to expand the application of robotics to animals and humans, it is necessary to prepare soft robots able to adapt to the environment in order to avoid damages to the organisms. Hydrogels are a promising material, as their mechanical properties can be tuned on demand, some of them present self-healing properties and they can be responsive to certain stimulus such as pH, light or electricity. [1]

Here we present a hydrogel, based on [2-(Acryloyloxy)ethyl]trimethylammonium chloride (AETA) monomer. This hydrogel is electrically responsive at 95% water content, producing a finger-like movement and a change in the hydrogel toughness when an electric field is applied. Unlike others electrically responsive hydrogels shown in literature, our gel doesn't need an external aqueous medium to move, which enables us to prepare electrically actuated soft robots outside water. [2]

However, it remains a challenge the preparation of a suitable electrode, flexible, conductive and stable enough to be used in soft robotics applications. Here we present recent advances in this kind of materials, by metal deposition over hydrogels which leads to flexible and highly conductive composites.

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M^a Prado Caballero

One-Component Iron Complexes for the Synthesis of Industrial Products



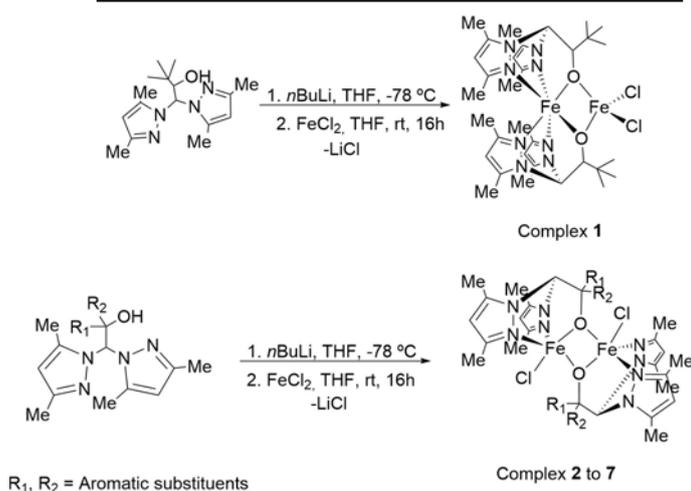
1. Introduction

Emissions of carbon dioxide as a consequence of human activity over the last two hundred years have resulted in a huge accumulation of this in the atmosphere which influences in global warming.[1] In this context, the atom-efficient reaction of CO₂ and epoxides for the preparation of cyclic organic carbonates and different polymers is an attractive option in terms of sustainability and atom-economy. Bifunctional metal systems have been far less studied for the synthesis of cyclic carbonates. [2] Iron-based catalyst systems have recently been gaining attention for these reactions because of their low cost, abundance, and reduced toxicity in comparison to other metal-based catalytic systems. In this work, we design new iron catalytic systems that behave as neutral bifunctional systems that show high catalytic activity for the fixation of CO₂ into cyclic carbonates under mild reaction conditions. In addition, these iron catalysts have shown excellent catalytic activity for the synthesis of fully bio-renewable cyclic carbonates and bio-based polymers.

2. Experimental Section

A family of halide Iron(II) complexes were synthesized from derived bis(3,5-dimethylpyrazolyl)methane based heteroscorpionate ligand. For these complexes, two dinuclear geometries are observed. For complex 1, which contains a heteroscorpionate ligand with *tert*-butyl group a dinuclear structure with two different geometries around iron centres is observed. On the other hand, Iron complexes with aromatic substituents (2-7) in the ligand have shown a symmetrical structure for both iron centres (Scheme 1).

The paramagnetic behaviour of iron complexes allows us the use of techniques based on Mössbauer spectroscopy and magnetism studies to determine the structure of both complexes, which were corroborated by X-Ray Diffraction.



Scheme 1. General synthesis of Iron (II) complexes

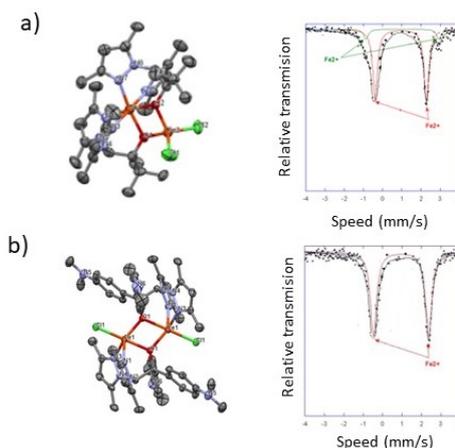
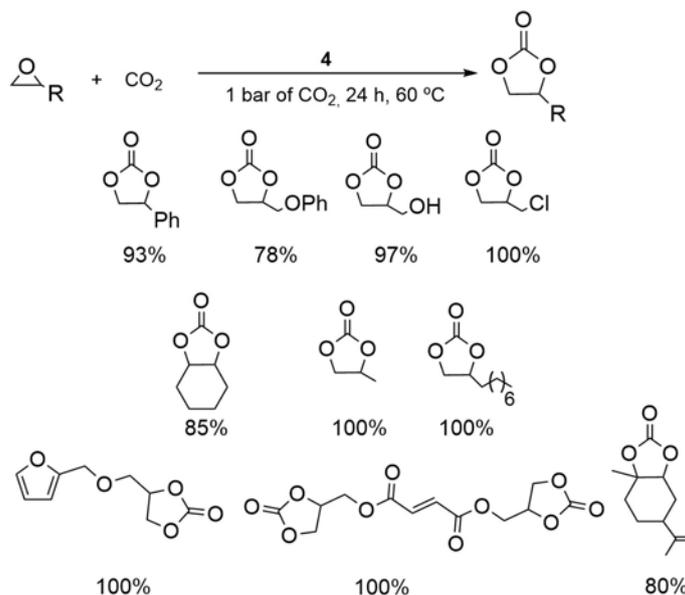


Figure 1. ORTEP views and Mössbauer spectra for: (a) Complex 1 and (b) Complex 5.

3. Results and Discussion

In order to determine the catalytic activity, several iron complexes were studied in the synthesis of cyclic carbonates from terminal epoxides. Under mild reaction conditions, one bar of carbon dioxide pressure, good conversions were obtained in presence of catalyst 4, in absence of cocatalyst and reaction solvent. In the optimal reaction conditions, a wide range of heterocycle-compounds were obtained from terminal and internal epoxides. Some of them come from natural resources, such as furfural, fumaric acid and limonene (Scheme 2).



Scheme 2. Synthesis of cyclic carbonates catalysed by complex 4.

For the purpose of studying the nature of oxidation state of iron centres in the synthesis of cyclic carbonates, it was decided to prepare a family of air-stable iron (III) chloride and bromide complexes. These new catalysts were studied in the synthesis of new polymeric materials such as polyesters. Some of them have been synthesised for the first time in this work.

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Rodrigo Oliver-Simancas

Mango by-Products: From Waste to Functional Ingredients



Mango (*Mangifera indica*) is the most harvested tropical fruit in the world and its processing activities generates unavoidable quantities of by-products, which are intrinsically rich in techno- and bioactive compounds. Since mango by-products have demonstrated to be a valuable source of bioactive compounds with antiproliferative activities against several cancer cell lines (1), mango kernel extract were tested in vitro on glioblastoma multiforme T98 and A172 cell lines and also nanoencapsulations of this extract have been developed to analyze its potential as a cosmeceutical ingredient to treat various skin conditions such as ageing or psoriasis.

Results showed that treatment with mango kernel extract (from 10 to 50 $\mu\text{g/ml}$ at 72 h) was the most effective inhibiting cell proliferation in both lines tested, reaching up to 70 % of growth inhibition. Fluorescent microscopy showed dose-dependent deterioration of certain cellular structures, such as the nucleus (Hoescht 33342 dye), as well as the activation of astrogliosis processes (GFAP dye). These results suggests that Mango Kernel Extract might be a promising agent for the treatment of glioblastoma multiforme. In terms of nanovehiculization, all the formulations were executed using soy lecithin as encapsulating lipid and water as dispersant agent. The best performing formulations in terms of particle characteristics, bioactivity potential and skin penetration and diffusion were those containing 20% glycerol and 10% propylenglycol (some these assays are already ongoing at the time of submission of this abstract). Overall, these research lay the groundwork for future researches in which in vivo together with clinical studies should be carried out to evaluate the translational performance of this fruit by-product extract.

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Daniel González

Gas-phase Reactivity at Ultra-low Temperatures for the Study of Interstellar Chemistry



Astrochemistry is a field which has experienced an enormous increase in the last decades due to the development of the radioastronomy which has made it possible that since 1937 more than 270 molecules (as of May 2022) have been detected in the interstellar medium (ISM) or circumstellar shells [1]. The discovery of this unexpected chemistry in the ISM has strengthened the exogenous synthesis hypothesis, in which the prebiotic molecules were synthesized in space and then, delivered to the Earth by meteorites, comets or asteroids [2]. Therefore, it is essential to study the chemistry present in the coldest regions (aprox. 10-100 K) of the ISM, known as dark clouds, which provide the raw material for solar systems. Astrochemical networks trying to model the IS chemistry have been improving with the inclusion of the rate coefficients (k) for the different processes, such as the bimolecular gas-phase reactions. k must be characterized under the appropriate temperature range (10-100 K) in laboratory experiments. For this reason, we have studied the gas-phase reactivity of two species found in the ISM, methylamine (CH_3NH_2) and ammonia (NH_3), towards an abundant IS radical, the hydroxyl radical (OH) between 11.7 and 177.5 K. It is important to know the processes involving these N-bearing species as their chemistry is closely linked to the simplest amino acid, glycine, observed in several comets [4] but undetected in the ISM so far. We have used the CRESU (French acronym for Reactions Kinetics in a Uniform Supersonic Flow) technique, based on supersonic expansions through a Laval nozzle, to experimentally determine k [3]. The OH radicals are generated by pulsed laser photolysis (PLP) of H_2O_2 and the OH temporal profile is monitored by laser-induced fluorescence (LIF). The results will be shown at the talk.

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Celia Gómez-Sacedón

A novel NiFe/NiFeO catalytic bilayer structure prepared by magnetron sputtering for hydrogen energy saving production via urea assisted water electrolysis

In this work different thin films as active catalyst-electrodes have been prepared by magnetron sputtering under oblique angle configuration for green hydrogen production via urea assisted water electrolysis. The films have been characterized by a number of surface analysis techniques and have been tested in half electrochemical cell and in a complete alkaline anion exchange membrane electrolyzer cell (AEM) using urea-water as feeding stream. In this way the oxygen evolution reaction (OER), which requires a high activation energy barrier, is replaced by the oxidation urea (UOR). This enables the hydrogen production at lower overpotentials (i.e., decreasing the energy requirements) and alleviates water contamination problems derived from industrial and urine rich effluents. Among the different prepared catalyst films: pure nickel, Ni/Fe mixture, and NiFe/NiFeO bi-layer, the latter one (Fig.1a) showed the best electrocatalytic performance. This electrode was selected as anode in a complete anion exchange membrane water electrolyzer (AEM) for urea oxidation, providing a decrease in 0.13 V in applied potential vs. the conventional water electrolysis to achieve $40 \text{ mA}\cdot\text{cm}^{-2}$. These operating conditions permit to produce hydrogen with a electrical energy demand of 47.18 kWh/KgH_2 , 8% less than for a conventional water electrolysis process. As a proof of concept, the system was coupled with a Photovoltaic Panel (PV) to demonstrate the long time and stable production of a pure hydrogen stream (Fig. 1b) via renewable energy.

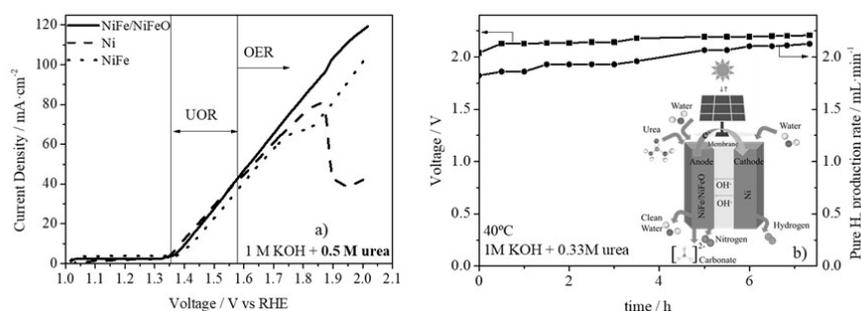


Figure 1. a) Linear sweep voltammetry experiments carried out in a solution of 0.5M urea with 1M potassium hydroxide in half electrochemical cell; b) Proof of concept of hydrogen production via direct PV-AEM coupling

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Eduardo Guisantes-Batán

Proteomic evaluation of intestinal function after dietary supplementation with grape seed polyphenols



Intestinal epithelial barrier has a crucial role in maintenance of the host homeostasis and bioactive compounds such as grape seed polyphenols has been related with lower incidence of many non-infectious diseases [1]. However, the effects of its dietary supplementation in gut homeostasis or its mechanism of action are not fully understood.

Thus, we evaluate the ileal proteome changes of young-healthy Wistar rats that were supplemented with a grape seed extract (GSE) (25 mg of GSE/kg body weight/day) for 28 days through SWATH-MS quantitative proteomics to gain insight into the molecular and cellular processes that were affected by this extract.

After GSE supplementation, 13 proteins were over-represented and 223 proteins under-represented in ileal proteomes. Attending to biological pathways, proteins implicated in intestinal motility and intestinal barrier integrity were over-represented in GSE-treated rats. Moreover, proteins related to energy metabolism, innate immune system and cancer development were under-represented, indicating that GSE supplementation at low doses may improve the intestinal barrier function and prevent aberrant over-activation of immune responses in the ileum.

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Daniel Alvarez

Anthropomorphic hydrogel-based phantoms for microwave imaging medical applications

Hydrogels are being widely used for biomedical applications based on their unique properties, commonly developed to mimic human tissues as image phantoms [1]. These phantoms are designed for medical imaging research, systems' characterization, and images' reconstruction optimization. The proposed work is ongoing for the optimized and valid use of dedicated hydrogel-based phantoms for breast microwave screening, a new medical imaging technique that exploits dielectric properties of tissues.

A literature review was performed to select the desired hydrogel's physical properties (mechanical and dielectric) based on updated data from breast tissues' experimental studies. A full dielectric characterization (to study conductivity and permittivity) of some hydrogel composites based on different monomers were performed via an open-ended coaxial probe [2]. Then, several theoretical models were implemented to reconstruct the dielectric parameters of common breast tissues (skin, adipose, glandular, cancerous) and compare them with measured hydrogels' dielectric properties. Additionally, models for hydrogels 3D printing are on development, based on real human breasts via MRI morphology features' extraction. An optimization of hydrogels' 3D printing is ongoing to assure and keep breast complex morphologies represented by used hydrogels.

Water-content stability, multilayered disposition and dedicated hydrogel-based representation of breast tumors are being studied via different phantom prototypes, which will be studied soon through an operational microwave imaging system.

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María Asensio

Kinetic study of the Cl atom reaction of biogenic aldehydes in the atmosphere

Aldehydes are volatile organic compounds (VOCs) recognized as primary and secondary pollutants emitted into the lower atmosphere from several sources. Large quantities of aldehydes are directly emitted into the atmosphere from biogenic and anthropogenic sources and are also formed in situ through atmospheric photooxidation reactions of other VOCs¹. These carbonyl compounds can be removed by tropospheric oxidation initiated by OH radicals (in the day-time), NO₃ radicals (in the night-time), and by Cl atoms (in the marine environment and coastal areas), being important contributors to the formation of peroxyacyl nitrates (PANs), ozone, and other compounds that have a detrimental effect on the environment and human health². Even at low levels, Cl atoms can have a profound impact on tropospheric oxidation, reacting faster with VOCs in comparison to OH. For this reason, in this work we report the gas-phase kinetic study at ground level conditions (T = 298±2K and P = 760±5 Torr of air) of the reactions between Cl and a series of aldehydes (2-methylbutanal, trans-2-methyl-2-butenal, 2-methylpentanal and 2-methyl-2-pentenal). For that purpose, an atmospheric simulation chamber coupled to a Fourier Transform Infrared spectrometer was used to determine kCl by a relative kinetic method³ in which Cl atoms were generated by photodissociation of Cl₂ by using actinic UV lamps (λ=340-400 nm). Finally, the atmospheric implications of the degradation of these aldehydes will be discussed in terms of its lifetime due to homogeneous reaction with Cl atoms, OH and NO₃ radicals.

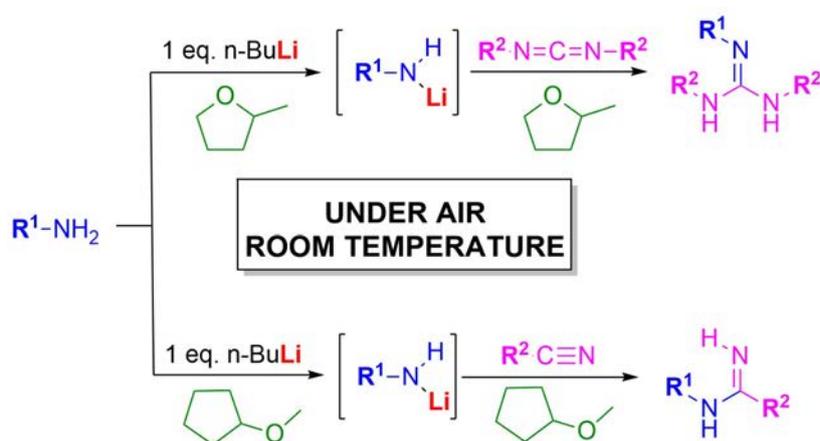
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Blanca Parra-Cadenas

Organolithium Chemistry under Sustainable Conditions: Synthesis of Amidines and Guanidines

The possibility of using organolithium compounds under-air opens the door to a greener polar organometallic chemistry.[1] In basis to our previous experience in the synthesis of guanidines and amidines,[2] in this work we describe the highly-efficient and selective fast addition of in-situ generated lithium amides $[\text{LiN}(\text{H})\text{R}]$ (obtained via acid-base reaction between $n\text{-BuLi}$ and the desired amine) into carbodiimides ($\text{R-N}=\text{C}=\text{N-R}$) or nitriles ($\text{R-C}\equiv\text{N}$), in 2-MeTHF or methylcyclopentylether as ethereal green solvents, at room temperature and in the absence of a protective atmosphere. This alternative synthetic methodology allows the straightforward and successful synthesis of either guanidines or amidines, without the need of isolation or purification steps of any halfway reaction intermediate. The robustness of the method allows the reaction to be carried out on a multigram scale, thus proving that our new and environmentally friendly protocol is amenable for a possible applied synthesis of these highly substituted iminic-type fine chemical products under bench-type reaction conditions.[3]



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Irene Acosta

Effects of Ultrasounds as a Pretreatment in Bioleaching of High Polluted Multi-Metal Mine Tailings

The mining industry has produced a vast number of hazardous wastes, which remain abandoned. These wastes combined with the climatic agents lead to the pollution of the soils, water, air, and biota nearby. In Spain, there are 75 abandoned mining sites considered of high risk for human health and the ecosystem. In this research, the used mine tailings were collected from the abandoned Pb/Zn mine of San Quintin Ciudad Real, Spain.

Bioleaching is a process by which an effluent with the metal pollutants of the tailings can be obtained, taking advantage of the microbial remediation. The inconvenience of this process is its slow rate and low yield, most specially compared with other hydrometallurgical process, less ecological but more effective. By the coupling of bioleaching with ultrasounds, we expected to achieve an increase in the overall reaction rate and metal recovery. [1]

The experiments were carried out at laboratory scale. The strategy was the biostimulation of the autochthonous microorganisms of the mine tailings, therefore conditions were set for the optimal growth. The procedure consisted in two steps, first discontinuous dosages of ultrasounds were applied; next the flasks were incubated at 30 °C and 150 rpm for 30 days. Two frequencies of ultrasounds were applied (37 kHz and 80 kHz) and different energy dosages (0 – 18 kJ/g).

The use of ultrasounds in this biological process showed a double effect of stimulating but also damaging the microorganisms. The main leached metals were iron (Fe), aluminium (Al) and zinc (Zn). Thus, increasing the energy dosage, the metal extraction incremented until the damaging effect was higher than the stimulating. Once this border was overpassed, the metal extraction decreased for both frequencies.

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Irene San Millán

Chitosan hydrogels: tissue engineering applications and magnetic properties

The field of tissue engineering has the potential to transform how we treat pathologies and diseases that cause tissue damage, by repairing, regenerating or improving the function of the damaged tissue. A key concept in tissue engineering is the use of biomaterials to support the growth of new cells and promote repair. Of the many types of materials that have been used in tissue engineering, hydrogels have emerged as one of the most prominent and versatile. Hydrogels can be designed to support cell proliferation, migration and differentiation, to permit oxygen and nutrient transport, and to provide cells with a 3D, highly hydrated environment that mimics native soft tissues. Careful design of the underlying polymer scaffold is therefore vital, dictating both the physical and biological properties of a hydrogel.

In this work, we highlight chitosan-based hydrogels as suitable scaffolds for tissue engineering applications (Figure 1). Chitosan is a partially deacetylated form of chitin and it occupies a distinct position amongst other biomaterials due to its abundance, versatility, biocompatibility and antimicrobial properties [1]. To increase the mechanical strength and structural integrity of this biomaterial, we have introduced acrylamide as a copolymer. Besides, the addition of nanomaterials such as graphene [2] and magnetic nanoparticles [3] will allow us to tune the biological response of cell cultures in our scaffold by increasing cell adhesion and controlling cell fate using external stimulation.

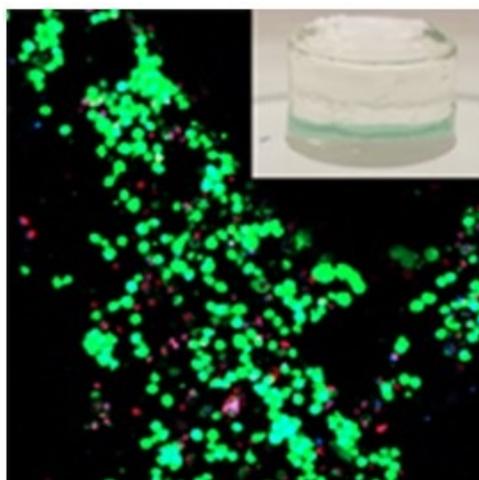


Figure 1. Cell culture in chitosan hydrogels.

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Rafael Delgado-García

Permalloy thin films on V-groove patterned substrates for sensing and biological applications

The magnetic properties of advanced materials, such as soft magnetic nano-undulated films [1], offer innovative possibilities for sensing and biological applications. For example, the morphologic and anisotropic characteristics of magnetic-coated V-groove substrates could be used for measuring perpendicular magnetic fields or guided control of cell movement [2].

For this purpose, Permalloy (Py) thin films were grown in V-groove (VG) patterned silicon substrates. Silicon substrates were processed through a multistep procedure involving photolithography, laser interference and reactive ion-etching techniques. The resulting pattern ($p=250$ nm, $\theta=55^\circ$) was characterised using SEM [Figure 1]. Permalloy thin films were deposited by DC sputtering with normal incidence on several substrates at a 1.6 \AA/s deposition rate.

The deposited Py-VG thin films were characterised using scanning probe microscopies and a vectorial Kerr magnetometer for the study of the resulting morphology and magnetic anisotropy.

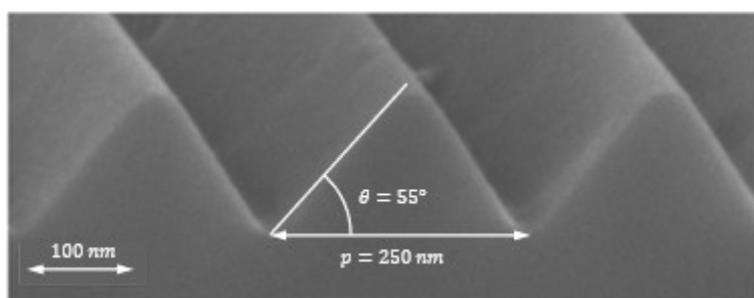


Figure 1. SEM characterization of nanopatterned V-groove silicon substrate.

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Daniela Berrios

Formulation of a nano biofertilizer based on soil yeast and its effects on lettuce crop: Preliminary results

Conventional agriculture uses large volumes of agrochemicals, which affects living organisms and ecosystems. Worldwide, agriculture has focused on reducing the use of agrochemicals, improving safety for the population and environment and reducing their costs without affecting crop quality. Nanotechnology, especially nanoparticles, offers an alternative for the sustainable development of agroecosystems. Currently, nano fertilizers, encapsulated agrochemicals and plant growth nano-promoters, have been developed, with potential applications for agriculture. In addition, with this new technology, nature-based alternatives have been developed, where soil microorganisms play an important role in the search for adaptation and mitigation strategies, such as abiotic stress. Soil yeasts are microorganisms that offer an alternative as potential plant growth promoters (PGP) through different pathways, alleviating alterations in root architecture, translocation of macro and micronutrients, improving photosynthetic activity, between others, in different crops such as lettuce, one of the most consumed crops worldwide, considered a healthy food, due to their content as antioxidant compounds and fiber.

This research is based on the development of a nano biofertilizer, composed by nanoparticles and soil yeasts. A completely randomized 4x2 design was developed, and two strains *Candida guilliermondi* and *Rodothorula mucilaginosa*, and with and without nanoparticle addition. PGP activities as siderophore production, phosphate solubilization and indole acetic acid were evaluated by spectrophotometric methods. Physiological parameters as stomatal conductance, water use efficiency, internal CO₂ concentration in leaves, photosynthetic rate and fluorescence were also evaluated. The main results of the PGP activities were the presence of siderophores, phosphate solubilization and indole acetic acid production, in both strains. In terms of growth, there are clear visual differences between strains and nanoparticle application. Finally, nano biofertilizers based on yeast has better efficacy in the presence of nanoparticle, with a potential improvement of the physiological and hydric status of crops.

Acknowledgments: FONDECYT 1190585 Project.

[Enlace video](#)

María Osorio-Alises

Studying the aromatic profile of dealcoholized rosé wines of the Cencibel variety

Recently, an increased ethanol concentration in wines has been observed, mainly because of climate change. On the other hand, consumers are increasingly demanding wines with reduced or null alcohol content due to the negative effects that it has in health. In this context, the winemaking industry has developed different techniques to reduce alcohol content in wine, among which post-fermentation techniques stand out because they are the ones that least modify the sensory profile of the wines. In this way, we have analyzed three rosé Cencibel wines with different alcohol content (control wine with a normal ethanol content, partially fermented wine and a dealcoholized "wine") in order to determine the main impact compounds and aromatic series of the aroma of the three studied wines, as well as to determine if the partial or total dealcoholization process produces changes in these profiles.

Volatile components were analysed by GC-MS with a previous isolation by solid phase extraction (SPE) [1]. Once the compounds were identified and quantified, the active aroma value (OAV = c/t) was calculated for each of them. In addition, aromatic descriptors were assigned to each of the compounds, allowing us to group those with similar descriptors into aromatic series. The intensity of each series was calculated as the sum of the VAOs of all compounds assigned to each of the aromatic series. Out of the 26 compounds with a OAV > 0.1, only some of them were found in concentrations above their corresponding olfactory perception threshold, so these were the compounds that were considered potential contributors to wine bouquet (acetaldehyde, ethyl octanoate, isoamyl acetate, ethyl butyrate, β -damascenone, etc.). The main aromatic series that determined the bouquet of the wines, regardless of the winemaking process, were the same (fruity, fatty and sweet), showing only differences in their intensity. The dealcoholized "wine" was the one that presented the lowest intensities of the sweet and fruity series, probably due to the lower concentration of esters.

We can conclude that dealcoholization process does not modify the aromatic composition of the wine, but it does affect the intensity of the profile.

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[Enlace video](#)

Noelia Viveros

What exists inside a beehive?

At present, beekeeping occupies a very representative place in the agri-food sector, with the products obtained emerging with increasing force, both in the national market and in the international market under the idiosyncrasy of "clean technology", propitiating an increase in demand by new consumers, concerned about a healthy life and a respect for the environment [1]. Inside a hive the main products found are: honey, pollen, royal jelly and propolis. Since ancient times, all of them have been used for their medicinal and nutritional properties, being recognized for their benefits in pollination and indirect pest control by competing with insects for plant food (nectar and pollen) [2].

Materials and methods

In order to know the microorganisms that are found both in the beekeeping environment (surface of the hive, atmosphere, bees and flowers) and in the products generated (honey, pollen and honeycomb), a sampling has been carried out in 4 apiaries and in a total of 23 honeys of different varieties. A count of bacteria, yeasts and molds has been carried out, taking 5 g of previously homogenized honey together with 45 ml of YPD broth (Yeast Peptone Dextrose) in a sterile flask. For ambient samples, the amount of sample is weighed and the same volume of YPD broth is added to make a 1:1 dilution in a stomacher bag. They were incubated with shaking (200 rpm) at 30°C for yeasts and molds and 37°C for bacteria for 24 hours. They were seeded on YPD agar and incubated at the same temperatures for 2/10 days. To carry out the identification of yeasts, the RAPD-PCR technique is performed together with the RFLP-PCR technique, thus identifying at the species level and the strain level. The databases used for the results of the two PCR techniques are Blast ® and Yeast-ID, respectively.

Results and discussion

The results obtained in the present work indicate that both in the environment and in the products of the beehives there is a growth of organisms, whose average counts obtained are 2.72 log cfu/g for bacteria and 0.84 log cfu/g for yeasts. Generally formed by bacteria of the genus *Bacillus*, and yeasts of the genus *Saccharomyces*, the most frequent being *S. bisporus*, *S. rouxii* and *S. bailii* and other non-*Saccharomyces* yeasts such as *Zygosaccharomyces* spp. and *Candida* spp. [3]. In addition, the presence of molds has been observed, which is associated with the intestinal content of bees, as well as with the environment, recognizing among them genera such as *Aspergillus*, *Chaetomium*, *Penicillium* and *Mucor* [2]. Finally, it should be noted that honey has been recognized as a source of *Clostridium botulinum* spores and is sometimes associated with ingested infant botulism [4].

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Enlace video

Tania Paniagua Martínez

Study of the capacity of fungal and bacterial laccases for the degradation of ochratoxin A in different reaction media

Introduction.

Ochratoxin A is a food toxin that can be found in different crops such as cereals, cocoa beans, coffee, grapes, etc. This toxin has nephrotoxic, immunosopressive, genotoxic, teratogenic, etc. effects, classified by the IARC as a possible human carcinogen. One of the methods of removing this toxin is the application of laccases of diverse nature on contaminated food. The presence of some compounds, which are called mediators, can intervene and improve the reaction of degradation of this toxin.

Objectives.

The main objective of this study was to evaluate and compare the effect of the laccases *Trametes versicolor* and *Lactobacillus casei* on the reduction of ochratoxin A in the presence of different mediators and in different reaction media.

Methodology.

Oxidation reactions were carried out in volumes of 100µL in microtubes of 1.5 mL. Duplicates of both the control samples and the degradation tests were performed. Some mediators used were phenolic compounds, such as catechin or ferulic acid. The reaction media used were sodium acetate buffer 50 mM at pH=4 and synthetic wine (12% ethanol and 5 g/L tartaric acid). The samples were prepared and subjected to a stirring reaction for 24 hours at 28°C. The reactions were stopped after this time by azide sodium 100 mM. The determination of ochratoxin A degradation was carried out using an HPLC coupled to a Q-TOF mass spectrometer.

Results.

The results showed that in the absence of a mediator there is no degradation of ochratoxin A, while in the presence of mediators such as catechin, epicatechin and ferulic acid significant degradation values are observed. On the other hand, the degradation values of this toxin were higher when the reaction medium was carried out in sodium acetate buffer.

Conclusions.

It can be concluded that these enzymes allow the reduction of the concentration of ochratoxin A under the conditions studied, always in the presence of a mediator. The influence of the reaction medium on the action of the different laccases was also confirmed.

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Claudia López Sánchez

Strategies for the synthesis and analytical control of Coenzyme Q10 nanoformulations

Nanoformulations have generated great interest in research due to their applications as carriers and bioactive release systems¹. This is the case of nanomicelles, which are used as colloidal nanocarriers based on surfactants that improve the bioavailability and solubility of lipophilic bioactives². For this reason, it emerges the need to apply analytical chemistry to improve the quality control of these nanoproducts as well as their identification, characterization, and quantification, through the development of new analytical methods and tools. For this purpose, Coenzyme Q10 nanomicelles were synthesized with two different surfactants (Kolliphor® HS15 y Tween 80®) by heating at 50°C in a water bath with constant stirring for 15 minutes. Then, a stabilizer consisting of 2% Glucose and 0.1538M NaCl was added, and the pH was adjusted to 4. These syntheses were characterized to compare the data with both surfactants, to optimize the CoQ10/surfactant ratio, to measure the encapsulation efficiency (%EE) of the bioactive, as well as the stability of the micelles and reproducibility of the synthesis. The characterization was carried out by absorption (UV-Visible) and emission (Fluorescence) spectroscopic techniques, dynamic light scattering (DLS), and scanning electron microscopy (SEM). Once optimized, the 1:10 ratio was chosen as the average size (18.76±1.39 nm and 176.70±2.65 nm obtained with Kolliphor® HS15 and Tween 80®, respectively) and polydispersity (0.21±0.05 and 0.09±0.04 obtained with Kolliphor® HS15 and Tween 80®, respectively). As for the encapsulation efficiency, it turned out to be 96.28% and 95.15% for the micelles formed with Kolliphor® HS15 and Tween 80®, respectively. Finally, according to their UV-vis and fluorescence spectra, as well as their sizes and polydispersity, measured for 1 month, the nanomicelles were relatively stable and reproducible.

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[Enlace video](#)

Esther Pinilla-Peñalver

Enhanced separation of seven biologically active compounds by capillary electrophoresis with carbon-based nanoparticles as additive

Biologically active compounds can be defined as nutrients and non-nutrients present in food matrices. These compounds are characterized by influencing cellular and physiological activities, showing a beneficial effect for health related to disease prevention and even forming part of therapeutic treatments [1]. In view of the growing worldwide usage associated with their health benefits, their efficacy and safety, sensitive and selective analytical methods are required for the determination of such food components and those related compounds that nullify the beneficial effects [2]. Herein, a highly reliable separation and determination of various health-promoter compounds was achieved by capillary electrophoresis (CE) based on β -cyclodextrin-functionalized graphene quantum dots (β cd-GQDs) as the background electrolyte additive. β cd-GQDs was successfully prepared and characterized for the first time, showing to enhance the separation efficiency of all the analytes studied, as the result of decreasing their apparent mobility and increasing their migration time. Up to eight consecutive runs were acquired with high precision for the separation of resveratrol, pyridoxine, riboflavin, catechin, ascorbic acid, quercetin, curcumin and even of several of their structural analogues. Baseline separation was achieved within just 13 min as a result of the effective mobility of the analytes along the capillary owing to the differential interaction with the additive. By the proposed analytical method, detection limits lower than $0.3 \mu\text{g mL}^{-1}$ and precision values were in the range of 2.1 – 4.0% for all analytes. The usefulness of the GQDs-assisted selectivity-enhanced CE method was verified by the analysis of food and dietary supplements. The applicability to such complex matrices and the easy and low-cost GQDs preparation opens the door for routine analyses of food and natural products.

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[Enlace video](#)

Andrea N. Arias

Comparative Study between Packed Column and Venturi in the Electro-absorption Process for the Removal of Xylene from Gaseous Streams

Volatile organic compounds (VOCs) are considered useful raw materials in several industries, especially in the production of paints and solvents. Xylene is used as a solvent and forms part of fossil fuels due to its high octane rating. In organic chemistry, it is used as starting product in the production of phthalic acids. However, it generates polluted gaseous streams that pose a major environmental problem associated with tropospheric chemistry, air quality and human health [1]. Electro-absorption is a novel technology to remove VOCs, such as xylene, from gaseous streams. It combines two stages: absorption in which pollutants pass from the gas to the liquid electrolyte and electro-oxidation where the elimination of them is carried out by oxidation reactions [2]. This study is focused on the evaluation of the electro-absorption process as a novelty treatment for gaseous streams polluted by xylene. To do this, two configurations in absorption steep were used: packed column and venturi, and it was evaluated the influence of current intensity (10, 50 and 100 mA cm⁻²) in the concentration of the liquid phase and the mass flow of gaseous streams. The inlet gas flow used was 6 L h⁻¹. Results show that in xylene degradations there was obtained higher elimination percentage with the venturi configuration. In the liquid phase, tolualdehyde was identified as the principal intermediate aromatic compound, also there were generated carboxylic acids. However, their concentrations were not significant amounts, it could be established that mineralization is the principal way of xylene in the electro-oxidation process. Meanwhile, there was observed a reduction in the concentration of the pollutant in the outlet streams compared to the inlet ones. This data verifies that electro-absorption is a functional electrochemical application to remove xylene from gaseous streams. When the current density rises, the removal percentage increases but the degradation percentage relative to the energy consumption decreases. This energy efficiency behaviour occurs because mass transport is the limiting stage in the oxidation of diluted organic solutions. This information contributes to the understanding of the kinetics and reaction mechanisms involved in the electro-absorption of xylene.

Acknowledgment

Financial support from the Spanish Ministry of Economy, Industry and Competitiveness, European Union through project PID2019-107271RB-I00 (AEI/FEDER, UE) is gratefully acknowledged. Andrea N. Arias acknowledge the FPI grant nº PRE2020-094902.

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[Enlace video](#)

Fernando Carrascosa

Reinforcement PLGA-Based Scaffolds Manufacturing via Supercritical CO₂ Foaming

Tissue engineering is an important field of regenerative medicine for tissue repair, particularly the repair of bone defects from trauma loss, tumor section, etc. Traditionally, bone implants have been made with metals or their alloys, but they are not absorbed by the body and require subsequent surgeries. In addition, they prevent bone regeneration due to the space they occupy. Therefore, the manufacture of porous scaffolds from biocompatible and biodegradable polymers, remains a great challenge.

Different polymers are postulated for this application, among them PLGA is one of the most used polymers for fabricating porous scaffolds. PLGA stands out as highly biodegradable and bioabsorbable polymer, in fact, it has been approved by the Food and Drug Administration.

However, one of the problems this polymer exhibits is poor mechanical strength [1]. Many studies have set their goals to reinforce these porous scaffolds by introducing reinforcing agents into the polymer matrix. Various compounds have been used as reinforcing agents as different calcium phosphates, Mg and derivates.

Among the manufacturing techniques for the preparation of polymeric scaffolds, the supercritical CO₂-assisted foaming offers significant advantages because is a solvent-free technique, since CO₂ is a gas non-toxic, chemically stable, non-flammable, and cost-effective. Additionally, CO₂ can achieve its supercritical state at “mild” conditions, T = 31 °C and P = 73 bar [2].

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J. Cencerrero

Nitrogen-doped graphene-based aerogels as electrocatalysts

The increase in CO₂ emissions and the excessive use of fossil fuels (coal, gas and oil) is forcing society to look for sustainable alternatives for obtaining energy. These alternatives are the renewable energies, and an established sustainable energy is the obtained from the energy vector “Hydrogen”. The producing of this molecule is being done by different methods, and a synthesis that obtains green and pure hydrogen is the Hydrogen Evolution Reaction (HER). Traditionally, this reaction has been catalyzed by noble metal catalysts (Pt or Pd) but their high prize and limited availability is an industrial handicap. Nowadays the studies are focused on develop new metal-free electrocatalysts with sustainable materials, such as graphene. The structure of the catalyst is relevant because it involves the active surface area, so the production of materials with high surface area and a well-defined 3D matrix structure is crucial, such as the aerogel disposition. Furthermore, if the graphene-based catalyst is doped with heteroatoms as nitrogen, the physicochemical properties of material change and it generates an n-type semiconductor which electroactivity increased.

In this study graphene-based electrocatalysts were synthesized by using non-nitrogenous (ethylene glycol) and nitrogenous reducing agents (hydrazine monohydrate, 2-chloroethylamine and ethylenediamine). The hydrothermal method was used to obtain the self-assembly of the graphene sheets, and then the freeze-drying generated the 3D carbon matrix. The electrocatalytic performance of the resulting graphene-based aerogels was strongly influenced by porosity, density, crystallinity and the crucial presence of nitrogenous and oxygenated groups. This work concluded that metal-free nitrogen-doped graphene-based aerogel synthesised achieved -12 mA cm⁻² at -0.15V (vs RHE) with 410 m²/g of surface area and a density of 0.0061 g/cc.

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[Enlace video](#)

Sergio E. Corriea

Use of electrogenerated ozone gas in PEM cells for disinfection of urine

The pollution of the aquatic environment constitutes one of the main problems in our society. In this context, pharmaceutical products have caused significant concern in the environmental field due to their frequent presence in effluent treatment plants (ETEs), with concentrations in the order of $\text{ng}\cdot\text{L}^{-1}$ to $\text{mg}\cdot\text{L}^{-1}$ [1]. Moreover, COVID pandemic events have demonstrated the necessity for advanced microbial decontamination as a preventative measure for epidemic control. Similarly, presence of SARS-CoV-2 RNA in urban wastewater has been reported [2]. Among these possible routes of entry to treatment plants, the main one is consumption and excretion in urine and feces. For this reason, it is necessary to develop clean and efficient technologies that reduce the danger from the environmental and health point of view before discharging them into the environment. Electrochemical Advanced Oxidation Processes (EAOP) can be considered a promising alternative. They can generate oxidants (such as ozone) currently used in the remediation of contaminated wastewater. With this background, this work evaluates, on the one hand, ozone electrogeneration by EAOP using boron-doped diamond (BDD) electrodes, and on the other hand, disinfection of hospital urine contaminated with *Klebsiella* by means of electrogenerated ozone gas. The influence of current density (25, 50 and $75 \text{ mA}\cdot\text{cm}^{-2}$) on ozone generation and elimination of *klebsiella* in synthetic urine was studied. The disinfection rate is higher when increasing the current intensity due to the higher production of ozone.

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Acknowledgements

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[Enlace video](#)

Leticia M. Da Silva

Generation of ClO_2 for Remediation of Soils Synthetically Contaminated with Carbamates

Soil pollution is a challenge that has involved researchers from different fields of science in search of technologies for their recovery. Thus, ex-situ soil washing appears as a simple and efficient solution for the remediation of contaminated soil. However, this treatment generates toxic effluents that cannot be discarded without treatment [1]. Given the need to treat this waste, there is another need to develop technologies capable of efficiently producing oxidizing species capable of completely removing dissolved organics. Among the wide variety of oxidants [2], the electrochemical production of chlorine dioxide from the reduction of chlorate (ClO_3^-) with hydrogen peroxide (H_2O_2), both continuously generated, is proposed in this work as an alternative for the treatment of effluents contaminated with carbamates. Thus, the first part of this work is to study the electrochemical production of ClO_3^- and H_2O_2 at a continuous flow rate, obtaining values of 2.67 mmol h^{-1} and 0.24 mmol h^{-1} with a flow rate of 0.1 L h^{-1} , respectively. This flow rate was chosen as the optimal to maximize the generation of the reagents (ClO_3^- and H_2O_2) responsible for the generation of ClO_2 . Another challenge of ClO_2 generation is finding the proper ratio of ClO_3^- to react with H_2O_2 . Since this reduction, it can also promote the formation of chlorite and hypochlorous acid, for example [3]. Hence, further studies should be carried out in order to quantify the generation of ClO_2 during the immediate reaction of ClO_3^- and H_2O_2 .

Acknowledgments

This work is part of the research project NEAT4SUST+PID2019-107271RB-I00 and Leticia Mirella da Silva also acknowledges the São Paulo Research Foundation (Processes 2021/06908-0, 2018/26475-9 and 2017/10118-0) for the Ph.D. sandwich scholarship.

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[Enlace video](#)

Yelitza Delgado

Treatment of Real Acid Mine Drainage for Metal and Energy Recovery by Electrodialysis and Bio-electrochemical Systems

Pollution is a serious problem that humans are increasingly aware, being one of them abandoned mines, which were used to extract metals in the last centuries. Nevertheless, when ores were exhausted, mines were abandoned irrespective of environmental hazard, polluting soil and water. Regarding water pollution, the effluent is named Acid Mine Drainage (AMD), being characterized by its high metal concentration and low pH. AMD treatment is needed both for ecological consequences and for the elevated valuable material contained, following circular economy recovering the metals. The real AMD (AMDR) that was utilized was from San Quintín mine (Ciudad Real, Spain).

In this research, two technologies were studied to treat AMDR. First, electrodialysis (ED) was used. Voltage and volume ratio between diluate and concentrated were the studied parameters with synthetic AMD (AMDS). Once these optimal conditions were selected, a test with them and AMDR was done. The obtained concentrated effluent was taken to posterior treatment with bio-electrochemical systems (BES).

Afterwards, bio-electrochemical systems treated the real concentrated effluent obtained by electrodialysis. Initially, MFC (Microbial Fuel Cell) configuration was used. The biofilm was on the carbon felt electrode in the anolyte. Biofilm creation lasted a month with growth medium and with activated sludge from a conventional wastewater treatment plan in Ciudad Real. In the catholyte occurred the electrodeposition of copper on the titanium electrode, reduction of Fe(III) to Fe(II) and production of energy.

MFC performance was operated for almost 300 h. Then, it was changed to MEC (Microbial Electrolysis Cell), applying 0.5 V for 48 h, 1.0 V for 96 h and 1.5 V for 96 h. Thanks to this configuration, reducing and recovering the rest of the metals was possible.

[Enlace video](#)

Rafael Granados

Production of oxidants in an electro-absorber designed by 3D printing for the degradation of benzene from gaseous streams polluted

The main objective of this work is the design of an integrated absorption column and electrochemical reactor in a single unit (electro-absorber) generated by 3D printing. Different materials for the fabrication of the electro-absorber were evaluated until getting a useful and contaminant-resistant prototype. A transparent resin was used allowed observe internal hydrodynamic features during the experiment. In this case, the electrodes used were Boron-Doped Diamond (BDD) and titanium for anode and cathode, respectively, sulfuric acid as electrolyte and absorbent, and benzene as a pollutant. A flow-rate gas inlet of 6.0 L h^{-1} and different current densities were tested (50 , 100 , and 150 mA cm^{-2}) and complete characterization of the liquid and gaseous phases were carried out by CG-MS. Benzene removal occurs by the production of a cocktail of oxidants during electrolysis in the electrochemical cell and by physical absorption itself. An evaluation of these oxidants of the liquid and gaseous phases were carried out by the standard iodometric titration method (Method I-/I₂)^{1,2}.

Acknowledgments:

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[Enlace video](#)

Hassay L. Medina-Díaz

Influence of Electric Fields (AC and DC) to Enhance Phytoextraction of Metals using *Lolium Perenne* from Multi-Metal Polluted Mine-Tailings

The presence of heavy metals in water and soils remains an important challenge being a risk for the environment and humans. The mining sector activities have led to the accumulation of mine tailings and other wastes abandoned and exposed to the environmental agents which contribute to the spread of pollution. Electro-phytoremediation emerges as interesting new technology for the treatment of polluted soil and rehabilitation of abandoned mining areas. This technology was tested in this research using real mine tailings. The experimental design was composed of 5 experimental series using ryegrass (*Lolium perenne*) as plant species and different types of the electric field that started to be applied 44 days after sowing and kept for 14 days with a voltage gradient of 1 V.cm^{-1} . The treatments were: alternate current with plants (EKPhAC) and without plants (EKAC), direct current with plants (EKPhDC) and without plants (EKDC), and plants without electric current (Ph). The physicochemical parameters were controlled in liquid samples from electrode wells, soil pore water, soil, and plant biomass. The reversal polarity mode in DC current treatment was efficient to avoid those extreme pH changes that could affect plant growth and rhizosphere development [1]. *Lolium perenne* grew up in highly polluted mine tailings. However, it showed phytotoxicity symptoms like chlorosis and early wilting in the growth period [2]. The metals accumulated to a higher extent in ryegrass tissues were Zn, Pb, and Cu. The application of electric current did not affect the biomass production of ryegrass. The application of alternate electric current (EKPhAC) improved mainly the metal bioavailability and uptake by *Lolium perenne*.

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Enlace video

Víctor Pertegal

Remove of antibiotic resistant bacteria on air with electrochemically oxidants generated

The research of biologic aerosols (bioaerosols) has increased strongly due to the world pandemic of SARS-CoV-2. The bioaerosols are suspended particle on the air whose size is in 0,1 to 100 μm and they expel them to the nose and/or the mouth of illness person when sneeze, talk or cough. These droplets in suspension can be constituted for diverse compounds of biological origin like bacteria, fungi or virus [1]. In this context, is very important to resalt the high frequency of hospital outbreaks for nosocomial infections that can be lethal and transmitted for airborne pathogens [2]. The nosocomial infections more frequent are the urine infections for bacteria like *Escherichia coli* or *Klebsiella* spp. And the respiratory infections for microorganisms like *Staphylococcus aureus*, *Legionella* spp. or *Aspergillus* spp., or viruses like respiratory syncytial virus. Have been used radiation technologies like the UV light, active filtration with HEPA filters or the fumigation with gas oxidants like ozone or hydrogen peroxide for control the extension of airborne pathogens [3]. In this study, the electrochemically technologies have been evaluated as alternative to conventional treatments. In a first step, the simulation of bioaerosols that contain *E. coli* will make in controlled conditions to laboratory scale using commercial hydraulic nebulizers commons and others more specific like the Collison nebulizer. To continue, the bioaerosols will recollect in a sterile liquid phase and they will treat direct or indirectly with electrochemically oxidants generated (ozone, hydrogen peroxide and chlorine dioxide). The production of this gas oxidants will develop with electrochemical cells capable of working to high pressure (until 10 bares) and with electrodes of flow through of them. In both cases, the ultraviolet light can be coupled to for knowing the synergic effect between treatment technologies.

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[Enlace video](#)

Álvaro Ramírez

Valorization of Polluted Vegetal Waste for Manufacturing Sustainable Cathode Materials for the Production of Hydrogen Peroxide

Electrochemical production of H_2O_2 is an area of research that has grown in importance in recent years due to the wide availability of this reagent and the high environmental impact of its production using traditional anthraquinone processes. The main direction of research is the cathodic production of H_2O_2 from oxygen reduction using carbonaceous materials, usually coated with a mixture of polytetrafluoroethylene (PTFE) and carbon black (CB) [1]. On the other hand, restoration of contaminated environments through electro-, bio-, and phytoremediation techniques is a viable alternative to restore large-scale contaminated sites. Nevertheless, the grown biomass accumulates the target pollutants and becomes a new contaminant.

In this context, this work proposes the utilization of heavy metal-contaminated plant biomass during phytoremediation of mining waste as a feedstock for the synthesis of carbonaceous materials that can be used as a substitute for CB for hydrogen peroxide production. This transformation is achieved by applying a hydrothermal carbonization (HTC) step to produce hydrochar that can be further transformed through thermal or chemical activation processes [2]. This approach, based on the concept of a circular economy, can simultaneously achieve two important milestones: recycling a wide range of polluting wastes and reducing the environmental impact of CB production influences.

Based on this, the HTC process and subsequent thermal activation were performed on *Spergularia* contaminated with Zn, Pb, and Cu to obtain materials with high specific surface area (around $400\text{ m}^2/\text{g}$) and high electrical conductivity. To correlate the properties of the material with the proposed application, structural and physicochemical characterizations, including thermogravimetric analysis, N_2 adsorption isotherms, surface conductivity, Raman spectroscopy, and elemental analysis, were performed. Finally, hydrogen peroxide production was evaluated with the most electrocatalytically active material in a continuous flow reactor with an electrode surface area of 64 cm^2 , comparing the hydrogen peroxide production efficiency of the synthetic material and commercial CB with successful results.

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[Enlace video](#)

Jesús Serrano

Electro-reforming of bioethanol streams produced by sugar fermentation on an optimized Pt-Ni anodic catalyst supported on graphene nanoplatelets

The continuous increment in gaseous pollutants has created the need to find new and cleaner ways to fulfill the global energy demand. In this sense, green hydrogen has gained importance as an energy carrier alternative to fossil fuels, since it can be obtained by alcohol electro-reforming in an electrolyzer. Ethanol is the main product obtained by the fermentation of carbohydrates from biomass¹. In ethanol electro-oxidation reaction (EOR), ethanol is oxidized in the anode, obtaining acetaldehyde, ethyl acetate and acetic acid; whereas the protons from EOR are reduced in the cathode into hydrogen.

Taking this into account, the electro-reforming of real bioethanol streams was performed in a Proton Exchange Membrane (PEM) electrolyzer containing a Membrane Electrode Assembly (MEA), in order to study the progress in ethanol production over fermentation time. The anodic catalyst employed was a 40 wt.% Pt-Ni (Pt/Ni 2/1) supported on graphene nanoplatelets, with an anode loading of 1.5 mgPt-Ni·cm⁻², as studied in a previous work of our group as a technical and economically appropriate alternative to commercial anodes. Then, three bioethanol streams were produced by fermentation at room temperature without stirring, with initial sugar concentrations of 150, 200 and 250 g·L⁻¹ and an initial dry yeast concentration of 5 g·L⁻¹. A general tendency in the increase in ethanol concentration given on each fermentation day was found as initial sugar concentration decreases. Conversely, larger ethanol yields and longer fermentation times were achieved as sugar concentration rises, achieving the 200 g·L⁻¹ bioethanol stream the best compromise between bioethanol production and fermentation time. Additionally, this stream accomplished the highest current density (~285 mA·cm⁻² at 1.2 V, on the 21st of fermentation), hence proving the promising use of this anodic catalyst in the electro-reforming of real bioethanol streams.

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[Enlace video](#)

Lais G. Vernasqui

Novel boron-doped diamond electrodes development for environmental applications

Electrochemical Advanced Oxidation Process (EAOPs) includes cheap and environmentally friendly methods with high efficiency in organic degradation with the production of highly oxidative species. In these techniques, although the hydroxyl radical is the main oxidizing formed agent, it can interact with other ions forming other oxidizing agents, which can be more stable than the hydroxyl radical. As they are multidisciplinary techniques, they depend on the knowledge such as material surface, electrochemistry, solid-state physics, and optics. Thus, EOPs are completely related to materials science. A material with a wide application in EAOPs is the boron-doped diamond (BDD). Its excellent mechanical properties, chemical stability, corrosion resistance, high oxidation potential, and low background current, make BDD a singular material for these applications. Besides, the methods of BDD growth allow the deposition above several substrates, ranging its grain size from micro to ultrananocrystalline morphologies. These different diamond composite properties can influence the pollutant degradation process as well as the oxidizing species generation, combining different morphologies and material characteristics to improve the final result. In this sense, we aimed at improving the BDD growth on porous materials by the deposition of novel boron-doped ultrananocrystalline on titanium dioxide nanotubes (TDN). From the perspective to grow diamond film from the chemical vapor deposition (CVD) technique, the porous substrate of the TDN is extremely advantageous, allowing to obtain a homogeneous film and distributed along the substrate to keep the substrate porosity motivated by the conversion of TiO_2 to TiC , which occurs in the diamond reactor. As result, we developed three different boron doped diamond electrodes that can be applied in EAOPs: 1) an ultrananocrystalline diamond electrode with porosity associated with TDN expose morphology and that presented photoresponse; 2) an ultrananocrystalline diamond electrode developed without seeding with the obtention of a homogeneous layer of diamond film that respects the porosity of the film and that have two different planes of diamond growth, also improving the electrode area; and 3) micro and ultrananocrystallines tridimensional diamond electrode grown on Ti grid with a titanium dioxide nanotube layer. All the electrodes were morphological, physical, and electrochemically characterized, proving their quality and potentiality for EAOP applications.

[Enlace video](#)

Jesús Fernández Cascán

Electrokinetic Remediation of DNAPL-Impacted Silt from Lindane Manufactures

Localización geográfica



RESIDUOS DE LINDANO EN SABIÑANIGO:

- ANTIGUA FACTORÍA DE INQUINOSA
- VERTEDERO DE SARDAS
- VERTEDERO DE BAILÍN
- EMBALSE DE SABIÑANIGO



Lindane
Gamma-HCH

25 kg

INGUNSA

[Enlace video](#)

O. Andrade

Optimizing the Supercritical Synthesis of TiO₂ Nanoparticles for CO₂ Photoconversion: Effect of Nature and Concentration of Ti Precursors

Photoreduction of CO₂ using solar energy and semiconductors such as TiO₂, ZnO, CdS, SiC or WO₃, is an alternative method to reduce emissions of this greenhouse gas. Within these materials, titanium dioxide (TiO₂) is one of the most widely used semiconductors for being efficient and nonthreatening for the environment [1]. One of the possibilities for obtaining these catalysts is to do it under supercritical conditions. Numerous studies have identified an improvement in the properties of catalysts synthesized in supercritical medium [1]. Using this technology, several studies have been carried out regarding the precursor for the synthesis process [2], but very few comparing the resulting physico-chemical characteristics, and fewer, comparing the effects of different ratios of hydrolytic agent (HA)/precursor [3]. For these reasons, this research focused on synthesizing catalysts with 4 different precursors, Diisopropoxytitanium bis (acetylacetonate) (TDB), Titanium (IV) isopropoxide (TIP), Titanium (IV) butoxide (TBO) and Titanium (IV) 2-ethylhexyloxide (TEO), and the HA/precursor ratio were 10, 20, 30 and 40 mol / mol. One of the variables observed is the yield production, where TIP and TBO presented a higher catalyst production (>70%). Also, TIP yield increased with increasing HA/precursor ratio. The physico-chemical characteristics vary differently according to the precursor and the HA/precursor ratio. Regarding the photocatalytic activity of the catalysts, TDB and TEO exhibit a higher production of CO and CH₄, but the influence of AH/precursor ratio was not apparent.

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Irene Guerra Velázquez

Synthesis and Formulation of Bio-Based Free-Isocyanate Polyurethanes

Over the years, the development of new materials that meet human needs in different applications fields, with the paradigm of the great climate and environmental concerns, has irremediably led the progress of technologies and production processes towards alternatives that are increasingly sustainable and respectful with our ecological-social environment.

Faced with the toxicological implications and environmental repercussions associated with certain materials such as traditional polyurethanes, polymers synthesized from isocyanates, sustainable alternatives arise to replace them in each and every one of their applications.

This project focuses on the study of the synthesis and formulation of isocyanate-free polyurethanes, also known as NIPUs, from a polyaddition reaction between raw materials of renewable origin such as carbonated soybean oil (CSBO) and diamines derived from dimerized fatty acids.

To do this, the optimization of the synthesis conditions and curing process of the materials is first studied, analyzing the influence of the molar ratio between reagents, temperature and curing time, setting the optimal conditions at 90°C, 6 hours and a molar ratio equal to 1.1.

Furthermore, it is proposed a modification of the chemical structure of the precursors through an original procedure that consist of the partial blocking of the active polymerization sites, thus allowing to obtain materials with a wide range of tailor-made properties. This study also allows to synthesize NIPUs with a 100% renewable origin, using as precursors CSBO and a reagent as simple and sustainable as water.

Finally, a foaming process assisted by supercritical CO₂ (scCO₂) is studied, which allows the reprocessing of the elastomers obtained previously and the obtaining of flexible NIPU foams, leaving the door open to further investigation on the optimal foaming conditions.

Alberto Moreno

Guanidines as catalysts for the reduction of CO₂ using hidroboranes

In last years, the scientific community has shown a huge interest for the use of CO₂ as C1 feedstock with the objective of reduce its concentration in the atmosphere. One of its most interesting transformations is the reduction into methanol, which can be used as fuel or as a building block to synthesise valuable chemicals.[1] To carry out this reduction, several reducing agents have been studied with homogeneous catalysts, where hydroboranes stand out for favoring mild reaction conditions and enabling the use of organocatalysts.[2]

In this work, we use four different trisubstituted guanidines [R¹-N=C(NHR²)(NHR³)] (R = aryl or alkyl groups) as catalysts for the reduction of CO₂ to methanol using two commercial hydroboranes (BH₃·SMe₂, 9-borabicyclo-[3:3:1]-borane (HBBN)) as reductant agents. Several experiments have been carried out to optimize the catalytic conditions, as well as catalysts' recycling experiments to prove their activity. Furthermore, stoichiometric experiments helped us to identify the intermediates of the catalytic reactions.

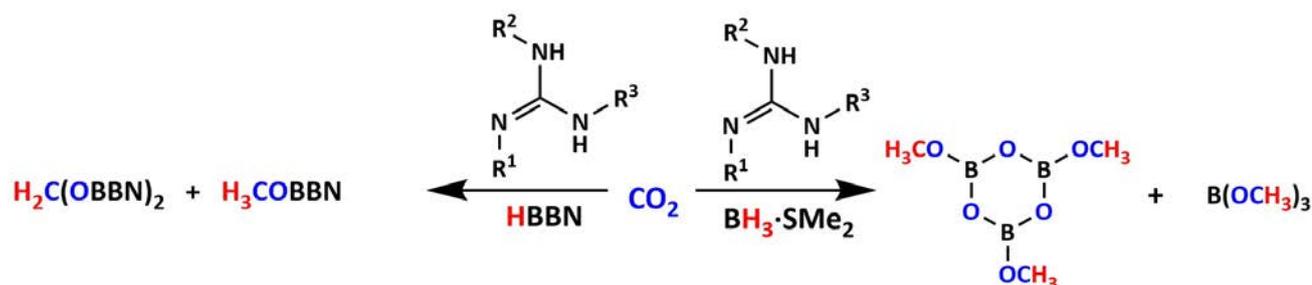


Figure 1: Catalytic reduction of CO₂ with HBBN and BH₃·SMe₂

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[Enlace video](#)

Antonio J. Troyano

Ruthenium (II) polypyridine complexes as potent PACT agents for selective therapy

The problematic of cancer as the second leading cause of death globally and the increase of antimicrobial resistance (AMR), due to ineffective treatments, have led to a wide variety of lines of research on novel pharmacological drugs to solve these issues. More effective and selective compounds are required to deal with the drawbacks of traditional chemotherapy: multidrug resistance and severe side effects. Photochemotherapy (PCT) has emerged as a promising therapy, a prodrug (usually named as photosensitizer) is used to treat the patient, this compound becomes active in presence of light while it remains innocuous in dark conditions. Photoactivated chemotherapy (PACT), which stems from PCT, uses a prodrug which suffers a photocleavage process (also known as photodissociation) when irradiated at a certain wavelength. This mechanism leads to one or more active species originated from the previous innocuous compound, which eventually triggers cellular death through an oxygen-independent mechanism. In this work, a series of ruthenium (II) compounds of formula $[Ru(tpy-R)(Me_2bpy)(L)]A_2$, potentially active as PACT agents, have been synthesized. The terpyridine ligand has been extensively studied as it gives unique electronic properties to the metal center, enhancing the photodissociation process. The 6,6'-dimethyl-2,2'-bipyridine (Me_2bpy) ligand generates a great steric hindrance produced by the methyl groups, improving photodissociation. The L ligand is a cytotoxic compound which is innocuous when caged in the metallic complex. Clotrimazole, an antifungal commercial drug, has showed interesting cytotoxic properties in several cancer cell lines. For this reason, it has been used as the cytotoxic compound (L).[1]

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[Enlace video](#)

Cristina Blasco-Navarro

Selective Formation of Highly Emitting Anthracene T-Shaped Excimers allows FLIM imaging in breast cancer cell lines

We recently reported a new anthracene-guanidine (AG) derivative able to form the rare T-shaped dimer in water solution, and where water molecules play a fundamental role assisting the self-assembly through H-bonds. Such T-shaped dimer formation is easy to be controlled, and stability depends mainly on the response to external stimuli: pH values within 4 – 10, water molar fraction ranging 0.8 – 1, and concentrations < 10 μM reinforce the stability enhancing luminescence properties - extremely high quantum yield ($\text{QY} \approx 1$) and maximum emission at 515 nm and large fluorescence lifetime (≈ 25 ns).

Next, we studied the behaviour of the AG dimers in biological systems, where different physiological factors such as the ionic strength, the presence of biological macromolecules, and the viscosity, among others, may affect their rate of formation or persistence. Fluorescence Lifetime Imaging Microscopy (FLIM) was used to monitoring populations of GA in human breast cancer (MCF7, BT474 and MDA-MB231). Different populations of monomer, T-shaped and π - π dimers were observed in the cell membrane, cytoplasm and nucleoplasm related to the local viscosity and presence of water (Figure 1). The T-shaped dimer is exclusively formed in the nucleus because of the higher density and viscosity compared to the cytoplasm. In addition, different rate of T-shaped to p-p dimer conversion was observed in the studied cell lines which would allow cell differentiation.

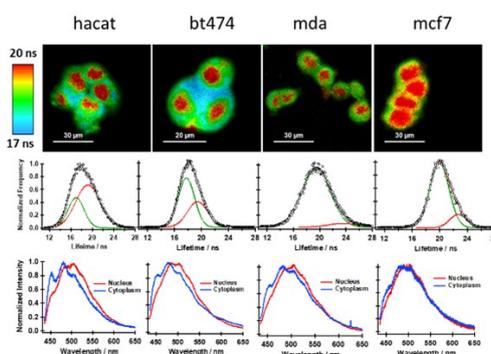


Figure 1. FLIM images of the studied cell lines along with the respective overall histograms of the average emission lifetimes and the emission spectra collected at selected points in the cell nuclei (red) and cytoplasm (blue).

[Enlace video](#)

Darío Martínez

Método de descomposición de dominios Schwarz para mejorar soluciones de colocación Legendre

Fluids are all around us, from gases to liquids. Therefore, it is important to understand them mathematically. The only way to study them nowadays is by numeric methods like Legendre collocation. Each numeric method has its own advantages and disadvantages. The Legendre collocation method is ill-conditioned, which means the computational complexity of the problem grows exponentially. The Schwarz decomposition method (SDM) is then used to overcome this issue. With SDM, the whole domain is split into several smaller subdomains where we can apply Legendre collocation independently. Thanks to SDM, we have been able to reach solutions never obtained before with a collocation method. The particular problem we are studying is the Rayleigh-Bénard problem, a fluid in a rectangular domain is heated from below keeping the upper tape at constant temperature. With the mathematical formulas there are two parameters that will define the fluid behaviour, the aspect ratio (Γ) and the Rayleigh number (Ra). Our main goal is to reach turbulence dynamics, which is a part of the field not very well known. Turbulence occurs with high Ra ($\sim 10^7$). With SDM and Legendre collocation Ra can be increased drastically. We are still studying these methods to their full potential, but the results already accomplished are very good and may be useful to show the huge impact SDM has alongside the Legendre collocation method.

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Enlace video

Jesús Cortés

A reduced order method for the Rayleigh-Bénard problem

Parametrized partial differential equations are standard tools to model many processes in scientific and industrial contexts. For this reason, understanding the solutions of such equations has become of paramount importance in the mathematical community. Two of the better-known techniques developed in this context are the numerical stability and bifurcation studies. However, performing such studies using a high-fidelity numerical scheme –finite difference method, finite element method or spectral techniques– has a huge computational cost, especially if fluid dynamics equations are involved. To overcome this problem, the mathematical community has developed several reduced order techniques, which allow to reduce dramatically the computational cost of stability and bifurcation studies.

Reduced order methods usually work in two steps. First, some solutions of the problem are obtained by a high-fidelity scheme. These solutions are processed to obtain a new basis of energetic solutions. Second, the solutions of the original problem are projected into the new basis. In this way, a new reduced order model is obtained, whose numerical evaluation is really fast, compared to that of the original problem.

In this communication we present a new reduction order technique applied to a classical problem in fluid dynamics: the Rayleigh-Bénard convection problem [1]. This fluid dynamics problem models the convection of a 2D fluid heated from below. Our reduction order technique follows the two steps listed in the above paragraph. The main novelty is the way solutions are obtained in the first step.

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[Enlace video](#)

Ana López-Hazas

Stimuli-Responsive Multi-Layered Hydrogels for Tissue Engineering

Hydrogels are three-dimensional networks of natural or synthetic polymers, capable of absorbing large amounts of water or biological fluids.¹ These systems are highly versatile due to their unique properties, which can be modified depending on the nature of the monomer units, the crosslinking agent or dopants molecules. One of the most promising applications of these systems is their use in tissue engineering for tissue and organ regeneration, bioactive molecules controlled release, living cells encapsulation or wound dressings among others.²

In particular, the aim of this research is the synthesis of a multi-layered hydrogel system consisting of two concentric layers: a magnetic synthetic hydrogel derived from 2-vinyl-4,6-diamino-1,3,5-triazine (DAT) surrounding a core with a biodegradable natural polymer of hyaluronic acid functionalized with methacrylic anhydride (HAMA) (Figure 1). This combination can be suitable, as the external magnetic field stimulus can induce the release of active molecules towards the inner natural hydrogel layer to stimulate cell proliferation and differentiation.

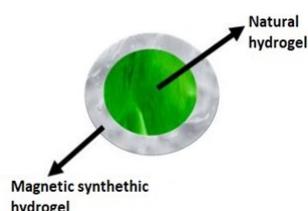


Figure 1. Bilayer hydrogel.

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[Enlace video](#)

Ana M. García

Nested supramolecular interactions: guest uptake in cages embedded in tripeptide gels

Supramolecular gels composed of short peptides are very popular thanks to their ease of preparation and their chemical diversity. The appropriate choice of amino acid chirality in D,L-tripeptides has emerged as a useful strategy to fine-tune the supramolecular behavior of these materials.[1] Metal-organic cages are interesting supramolecular structures able to selectively encapsulate guests for a wide variety of uses, including chemical separation between immiscible liquid phases.[2] In this work, we illustrate hybrid gels based on nested supramolecular interactions: guests can be separated from a mixture via encapsulation in their respective host cage embedded in discrete peptide gel phases (Fig. 1). These hybrid materials have been characterized by NMR, Raman, EDX, UV-visible and CD spectroscopies, TEM and rheology. Overall, this investigation represents a general strategy for the immobilization of supramolecular hosts within gels to yield novel materials that could be applied for molecule separation

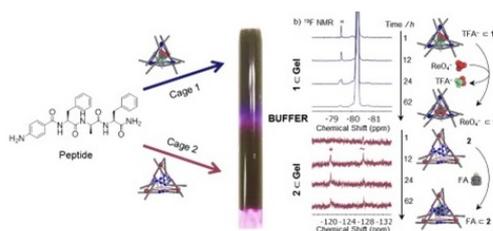


Figure 1. ^{19}F NMR spectra of 1 Gel (blue) and 2 Gel (pink) showing respectively the decrease of the encapsulated TFA^- peak ("u") and the increase of the both the encapsulated (*) and free (~) FA over time after addition of a mixture of 1 eq. or FA and ReO_4^- .

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[Enlace video](#)

Alicia Morcillo

Synthesis and characterization of self-healing materials

Soft materials such as polymers, elastomers or hydrogels can be easily damaged, for that reason their lifetime, in most of the cases, is too short. This problem has led to the study of self-healing materials.

In the last years, many materials with different self-healing mechanisms have been studied. The most important mechanisms are: i) encapsulation of self-healing agents, ii) metal-ligand coordination bonds, iii) reversible covalent bonds such as Diels-Alder reactions, iv) non covalent bonds such as hydrogen bonds or ionic interactions or hydrophobic interactions.¹

Some of the previous mechanisms are not autonomous, that means that the material must receive an external stimulus like light, heat, or an electromagnetic field in order to self-heal. For that reason, these materials do not have many applications.

The objective of this work is to find hydrogels with self-healing and with good mechanical properties. The starting point is the SHAP hydrogel (Self-Healing AETA-based Polymer),² this hydrogel was synthesized by the MSCO Nanochemistry group; it was synthesized by photopolymerization of (2-(Acryloyloxy)ethyl)trimethylammonium chloride (AETA) using N,N'-Methylenebisacrylamide (MBA) as the chemical crosslinker and sodium 2,4,6-trimethylbenzoylphosphonate (NaTPO) as photoinitiator using water as solvent. The self-healing capacity of this hydrogel is given by the hydrogen bonds that form the water molecules inside the structure. To improve the self-healing capacity of the SHAP hydrogel, monomers with diverse charges were added to the SHAP chemical structure producing an additional electrostatic interaction between the different monomers. Different hydrogels were synthesized using various types of negatives and positives monomers and different molar concentrations.

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Daniel Iglesias

Functionalized carbon nanohorns with SERS activity

In the last decades, organic chemists have developed numerous functionalization routes to fine tune the properties of carbon nanomaterials including carbon nanotubes, graphene, or carbon nanohorns. Carbon nanohorns are spherical aggregates of horn-shaped carbon nanotubes. Their size distribution, low toxicity and electrical properties make them very interesting for their application in sensing and bioimaging. This contribution will show the functionalization of carbon nanohorns with a series of thiophene derivatives and their potential use in Surface Enhanced Raman Spectroscopy (SERS).^{1,2} In particular, it will focus on the fast and efficient eco-friendly covalent functionalization of carbon nanohorns via the 1,3-dipolar cycloaddition and their unique spectroscopic features. The work combines experimental and in silico studies to understand the Raman enhancement.

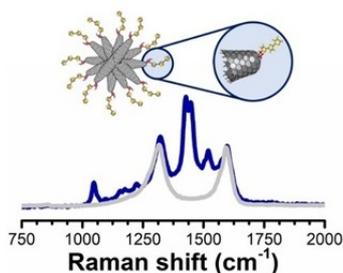


Figure 1. Schematic representation of covalently functionalized carbon nanohorns with thiophene derivatives and the comparison of the Raman spectra of the pristine and the functionalized materials.

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[Enlace video](#)

Francisco M. Soria

Design and Development of a HARD/SOFT Double Hydrogel System to Improve Reproductive Biotechnologies

Conventionally, cell culture is developed in 2D environments, which can affect the cell morphology, the communication between cells and with the extracellular matrix and cause several changes. In order to reduce cell culture and physiological environment, 3D scaffolds have been developed, partially maintaining the mechanical and biochemical cues of the original tissue. In particular, in vitro fertilization is usually also performed in 2D environments and half of the embryos fail to develop. In this project, we aim to create a 3D biocompatible scaffold for 3D cell culture by using hydrogels.

Hydrogels are three-dimensional polymeric materials chemically or physically cross-linked which can absorb water without dissolving in it. They are also very porous materials, which allows the exchange of nutrients and cellular wastes.^{1, 2}

Our scaffold consists of a natural part in the middle that will contain the oocyte, and another natural or synthetic part surrounding it, trying to mimic the natural environment of oocytes. The central part is made of alginate, which is highly biocompatible. The external part can be made of three different kinds of hydrogels: one of them is based on 2-Vinyl-4,6-diamino-1,3,5-triazine (VDT); the second one is based on sodium 4-vinylbenzenesulfonate (VBS) and the third one is based on a natural polymer, i.e., chitosan. These hydrogels can link to alginate through physical interactions.

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Enlace video

Irene Chacón

Synthesis of arylethyl pyrazine derivatives. Application as optical waveguides

Ever since it was shown that light could be confined in a medium¹ and travel through it carrying information,² research in this field has continued unabated. The goal is for photonics to overtake electronics in the world of communication because of its many advantages. In this sense, miniaturised photonic devices are being developed, for which the design and synthesis of optical waveguides, which are structures capable of efficiently propagating and confining light, is fundamental.³

In this work, four arylethynyl pyrazine derivatives have been synthesised, supramolecular aggregates have been formed using the slow diffusion technique, their morphology has been studied by SEM and those with the best structures have been measured as optical waveguides using a confocal fluorescence microscope. Three of the synthesised compounds have optical waveguide behaviour (Figure 1).



Figure 1. Arylethynyl pyrazine derivatives as optical waveguide.

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Enlace video

Irene Sánchez-Ajofrín

A Novel Bioinspired Hydrogel System Improves the Quality of Sheep Oocytes after in vitro Maturation

The global assisted reproductive technology (ART) market is expected to reach \$50.32 Billion in 2027 due to the increasing incidence of infertility and growing awareness. Despite being one of the most promising ARTs, oocyte in vitro maturation has become a major limiting factor for the in vitro production of viable embryos in different mammalian species.

To improve the standard in vitro models within oocyte maturation, we have developed a new 3D culture system based on binding two hydrogels that closely mimic the mechanical characteristics of the mammalian ovary. Thus, DNA fragmentation studies, confocal microscopy, and quantitative real-time PCR demonstrated that the double hydrogel system significantly improved the quality of matured sheep oocytes.

According to these results, the proposed system is potentially a novel tool for reproductive technologies and livestock production applications.

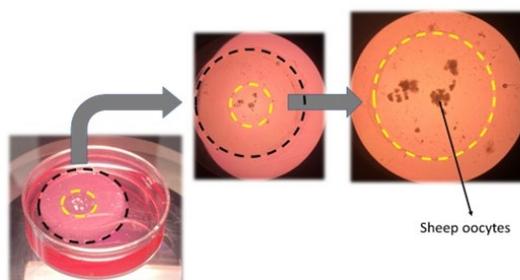


Figure 1. Novel hydrogel system during oocyte in vitro maturation

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Sara Gallardo

Microfluidics in Supramolecular Chemistry and Materials with Waveguide Properties

Microfluidics is the science of systems that employs small amounts of liquid or gaseous fluids, using channels ranging in size from tens to hundreds of micrometres. The high surface-to-volume ratio of microreactors enables a favored mass and heat transfer as well as an easy diffusion of molecules. The result is a reduction in analysis times, and low reagent consumption and production of undesirable by-products, reducing cost.

In this work, the advantages of this discipline have been used to study the occlusion of naproxen in the supramolecular hydrogel that forms the tripeptide LLeu-DPhe-DPhe using 3D printed microfluidic devices made of polydimethylsiloxane (PDMS). The waveguide property of this tripeptide is under study.

In addition, focused on preparing a hydrogel with waveguide properties to guide the light inside a microfluidic channel, we started preparing a macroscopic waveguide as first step. These structures are capable of confining and transmitting light through the total internal reflection (TIR) phenomenon and its importance deals because they represent the major component of photonic chips. For the synthesis of the materials, a 1,8-naphthalimide derivative (Fig. 1) has been synthesised, which is characterised by having excellent photostability, being a fluorophore unit, good structural flexibility and a large Stokes shift (a prerequisite to behave like an optical waveguide). A macroscopic organogel that contains the 1,8-naphthalimide derivate in its structure was also prepared. In addition, its waveguide property is under study.

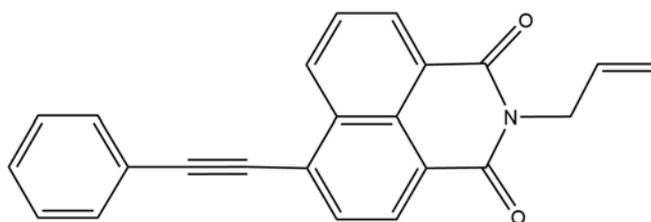


Figure 1. Chemical structure of the synthesised compound

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Viviana J. González

Synthesis of 2D nanomaterials with metallic nanoparticles

Different synthesis methods emerged over the years, first for graphene and then for other 2D nanomaterials. With the addition of nanoparticles, these materials can be tuned surface and properties [1] to enhance catalytic, magnetic, electrical, and optoelectronic properties [2]. These hybrid nanomaterials can be synthesized by solution mixing [3], sol-gel processes [4], microwave irradiation [5], etc. However, these methodologies have disadvantages, such as using hazardous and non-environmentally friendly reactants, time-consuming, and yields [6]. Here in a simple, one-step, and environmentally friendly methodology, we report a new ball milling procedure for synthesizing hybrid 2D nanomaterials (graphene to dichalcogenides) with metallic nanoparticles.

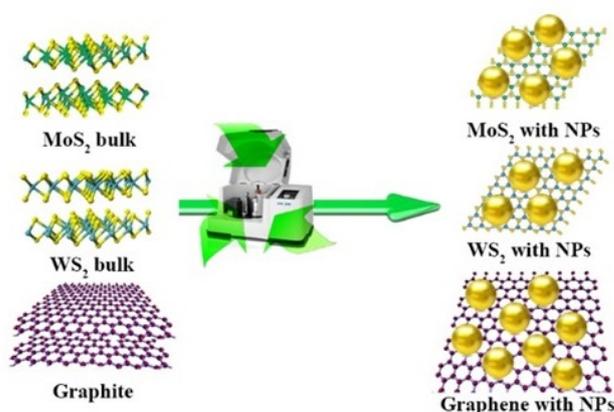


Figure 1. Synthesis of hybrid 2D nanomaterials.

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[Enlace video](#)

Aikaterini E. Xezonaki

Ultraviolet (UV) photolysis study of Furan-based compounds in the gas phase under exposure on solar radiation

Biomass burning (BB) due to wildfires, agricultural burning, and domestic fuel use are substantial both biogenic and anthropogenic sources of a series of volatile organic compounds that impact the air-quality and human health. Recent field studies^{1, 2} have measured a series of furanoids, at significant levels, despite their high tropospheric reactivity. Furans are heterocyclic, semi- or low-volatile oxygenated compounds that can be aromatic or not. Besides, their inherent toxicity furans atmospheric degradation could lead to ozone formation, a strong greenhouse gas and/or to secondary organic aerosols (SOAs) formation and thus a substantial source of the atmospheric particulate matter.³ The presence of the heteroatom on the five-member ring, along with the several optically active groups that have been proved to contain, e. g. carbonyl-, alkyl or alkoxy- groups, could make them potent UV absorbers in the actinic wavelength range. In this work, the UV photolysis of furan derivatives and the formation of oxidation products are being studied by exposing the furans on solar radiation using a solar simulator, as an irradiation source, and a proton transfer time-of-flight mass spectrometer to monitor the loss of furan compound and formation of gaseous products. The size-distribution of formed SOAs is monitored by a fast mobility particle sizer.⁴ The UV absorption cross sections are also determined in the UV actinic solar region ($\lambda > 290$ nm) in order to evaluate the UV absorption capability of these compounds and their potential atmospheric degradation by photolysis.

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[Enlace video](#)

Clara Inés Alcolado

Effects of the Oxidation of Salicylic Acid by Peroxynitrite

Non-opioid analgesics and non-steroidal anti-inflammatory drugs, such as salicylic acid derivatives are on the list of essential drugs of the Health Organization [1]. This compound has been the most prescribed against pain and inflammation [2]. Their biological action has been widely studied, however, their reaction at the intracellular level is not so well known. More specifically, there are hardly any studies on their possible mechanism of oxidation of these analgesics. On the other hand, peroxynitrite is an important pro-oxidant in the human body, this molecule is present in organs, tissues, cells... being the first defense at the cellular level against virus and bacterial infections.

Also, it is very important to understand the mechanism of salicylate degradation by peroxynitrite at cellular level. The experimental results have shown a complex order to peroxynitrite and salicylic acid concentrations (Fig. 1).

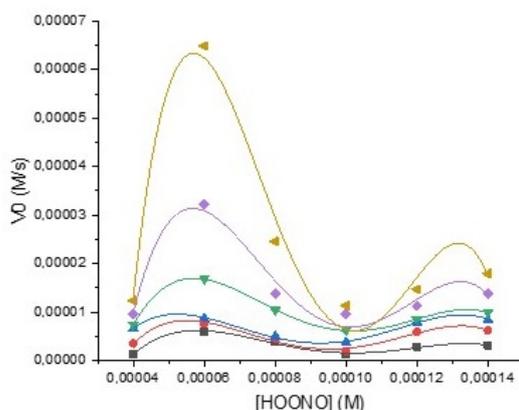


Figure 1. Initial rate versus oxidant concentration, at different substrate concentrations. Experimental conditions: $I = 0,15 \text{ M}$; $\text{pH} = 2$; $T^a = 25^\circ\text{C}$.

A thorough knowledge of this mechanism as well as of all intermediates and reaction products can improve their analgesic effect and reduce adverse effects.

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Daniel Alba-Elena

A new iodometric microwave assisted method for peroxide determination

Peroxides play an important atmospheric role both in the gas and particle phases. Several techniques are available in the literature to measure peroxides in Secondary Organic Aerosols (SOA), although current techniques are very expensive or time consuming. In the present work, a new fast and sensitive iodometric spectrophotometric method has been developed based on the traditional iodometric method (1-2). The proposed method is based on the acceleration by microwave radiation of the reaction of peroxides with potassium iodide in acid medium to liberate iodine, that in the presence of excess of iodide forms triiodide that could be monitored at three different wavelengths (287 nm, 351 nm y 420 nm).

Different analytical parameters including pH, potassium iodide mass, temperature and time of thermostatic bath, microwave power and time, interferences due to oxygen and metals were evaluated. The method has been optimized for H₂O₂ and t-butyl hydroperoxide (one of peroxides that reacts very slowly in the traditional method), in contrast with previous studies that only used H₂O₂ or an organic peroxide that reacts faster with iodide.

The main advantages of the new method in relation to the traditional method are the following: less time-consuming analysis, lower and controlled oxygen interferences, and smaller sensitivity differences between different peroxides.

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[Enlace video](#)

M^a Gabriela Viteri

Air quality assessment in the ecological area of Las Tablas de Daimiel National Park, in Spain

Air quality is generally measured in urban and industrial sites. Nevertheless, anthropogenic activities can also contribute to the pollution of natural areas. Although these areas may be far away from urban or industrial sites, remote transport of persistent pollutants to national parks or protected areas has been reported in previous studies [1,2]. This work shows that national parks and other protected natural areas require in situ tools to monitor and detect local and remote air pollution sources which are a threat to natural resources. The main objective of this work is to perform a field campaign inside a national park involving the measurement of the air criteria pollutants, O₃, NO₂, NO, SO₂, CO, PM_{2.5} and VOCs from anthropogenic sources and meteorological parameters to assess the air quality inside the park Las Tablas de Daimiel and to identify local or distant sources of pollutants which could endanger its preservation.

The study was carried out from March 2020 to July 2021, involving the continuous measurement of meteorological data, gaseous pollutants, and PM_{2.5} inside the park with one hour time resolution. Twelve campaigns, one week duration, were also performed to sample air in sorbent tubes to analyse VOCs. The results are discussed considering meteorology, especially wind and speed direction together with the assessment of back-trajectories of remote air masses. The results show that, excepting for the high levels of ozone, air quality in the park is slightly affected by local and remote air pollution sources.

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Enlace video

M^a Teresa Pinés

Addition of biomass combustion ashes in ceramic materials: influence on composition, properties and environmental aspects

In this work, it is analysed the influence of the addition of biomass ash, specifically olive pomace ash, on the properties of ceramic material. This possibility has been raised due to the high potassium content of these ashes and their possible behaviour as a fluxing material. They could be used as a substitute for alkaline feldspars, as these ashes have a potassium content 30% higher than that of feldspars (12-15%)^{1,2}.

To this end, physical, chemical and mineralogical analyses have been carried out in order to characterize the ashes to be used, the raw material clays and the ash-clay mixtures made in the laboratory (ash content 5% or less)³.

Fluorescence and X-ray diffraction studies, thermal methods such as thermogravimetry or optical heating microscopy have been carried out on the different raw materials and new mixtures. These studies carried out at laboratory level, together with the performance of tests at industrial level, will make possible to determine whether the ashes show fluxing behaviour⁴.

The results are related with i) the possibility to reduce the high firing temperatures of the ceramic production process, ii) the possible reduction of carbon dioxide emissions into the atmosphere, iii) the possible contamination or not by other compounds and iv) the assessment of the mechanical properties of the new mixtures produced.

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[Enlace video](#)

Sara Espinosa

Hydrofluoroethers as eco-friendly candidates for replacing greenhouse gases

Hydrofluoroethers (HFEs) have been proposed in the last decades as climate-friendly alternatives to potent greenhouse gases, such as hydrofluorocarbons, in several industrial applications (i.e: refrigerants, blowing agents, etc). Assessing the impact on climate change is indispensable to evaluate the suitability of HFEs as environmentally friendly candidates to replace high global-warming (GWP) species. To achieve that objective, it is necessary (1) to investigate the temperature and pressure dependence of the absolute rate coefficient, $k_{OH}(T,P)$, for the reaction of HFEs with OH radicals to mimic the tropospheric conditions, which is the main removal process in the atmosphere, and (2) to determine the IR absorption cross sections in the atmospheric window ($720-1250\text{ cm}^{-1}$). With these two parameters the GWP of HFEs can be estimated. In the present work, we present the first kinetic study of the OH-reactions with $\text{CF}_3\text{CH}_2\text{OCH}_3$ (HFE-36 263fb2), $\text{CHF}_2\text{CF}_2\text{CH}_2\text{OCH}_3$ (HFE-374pcf) and $\text{CF}_3\text{CF}_2\text{CH}_2\text{OCH}_3$ (HFE-365mcf3) as a function of temperature (263-353 K) and pressure (50-500 Torr of helium) using the pulsed laser photolysis/laser induced fluorescence technique [1]. No pressure dependence of the rate coefficient was observed in the studied range and the temperature dependences ($k_{OH}(T)$ in $\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$) are well described by the following Arrhenius expressions [1]: $k_{OH}(T) = (3.88 \pm 0.89) \times 10^{-12} \exp[-(508 \pm 69)/T]$ for HFE-263fb2, $k_{OH}(T) = (2.81 \pm 0.33) \times 10^{-12} \exp[-(312 \pm 35)/T]$ for HFE-374pcf and $k_{OH}(T) = (2.60 \pm 0.31) \times 10^{-12} \exp[-(319 \pm 35)/T]$ for HFE-365mcf3. From these results, the atmospheric lifetime (τ) for HFE-374pcf, HFE-263fb2, and HFE-365mcf3 due to the OH-reaction are 12, 17, and 13 days, respectively. Considering τ and the IR absorption cross sections determined in this work, the radiative for these HFEs were $0.03\text{ W m}^{-2}\text{ ppbv}^{-1}$. At a time horizon of 100 years, GWP relative to CO_2 for these HFEs results in the range of 0.40-0.76. [1] The drastic reduction in GWP observed with respect to the gases HFEs will replace minimize the effect on the global warming of the planet.

References

[1] Blázquez, S.; Espinosa, S.; Antiñolo, M.; Albaladejo, J. & Jiménez, E. Phys. Chem. Chem. Phys., 2022, published on line (DOI: 10.1039/d2cp00160h).

Enlace video

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