

The Royal Society of Chemistry and iCAST present

# Chemical feedstocks for sustainable industry

1st December 2023, Burlington House, London

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# Programme

**0900 – 0930 Registration & Coffee**

**0930 – 0945 Introduction**

**0945 – 1215 Session 1: Sustainable chemicals from biomass residues**

**0945 – 1015 IT1:** *Exploring cellulose water interactions for making composites;* Professor Steve Eichorn, University of Bristol, U.K.

**1015 – 1030 T1:** *Developing a novel ultrasonic biorefinery process and marketable biochemicals;* Miranda Lindsay-Fynn, Sonichem, U.K.

**1030 – 1045 IT2:** *Bio-derived compounds from easily accessed platform molecules;* Dr Rob McElroy, University of Lincoln, U.K.

**1045 – 1100 T2:** *Biosensors and biocatalysis for biorefinery;* Neil Dixon, University of Manchester, U.K.

**1100 – 1115 T3:** *Building a terpene-based biorefinery;* Josh Tibbetts, University of Bath, U.K.

**1115 – 1130 T4:** *Lignocellulosic biomass conversion into high-value biochemicals;* Mireia Mora, Universitat Autònoma de Barcelona, Spain.

**1130 – 1200 IT3:** *The intrinsic link between biomaterials and Net Zero;* Steven Brown, Scott Bader, U.K.

**1200 – 1315 Lunch & Posters**

**1315 – 1445 Session 2: Oleochemicals**

**1315 – 1345 IT4:** *Effect chemicals from waste bio-oils;* Professor David Cole-Hamilton, University of St Andrews, U.K.

**1345 – 1400 T5:** *Leveraging a green transition with oleochemicals: navigating regulatory landscapes, measuring sustainability, and fostering collaboration;* Jan-Domenic Urbas, HOBUM Oleochemicals, Germany.

**1400 – 1415 T6:** *Natural clay catalysts for processing sustainable chemical feedstocks;* Oscar Kelly, BYK Additives Ltd., U.K.

**1415 – 1445 IT5:** *The future of chemistry;* Tony Heslop, BASF, U.K.

**1445 – 1515 Tea & Posters**

**1515 – 1700 Session 3: End-of-life plastic recycling**

**1515 – 1545 IT6:** *Catalytic upgrading of polymers – is chemical recycling the answer?;* Professor Matthew Jones, University of Bath, U.K.

**1545 – 1600 T7:** *Combining enzyme surface modification and ionic liquids for a facile strategy to enhance biocatalytic degradation of plastics;* Alex Brogan, King's College London, U.K.

**1600 – 1615 IT7:** *IP trends in the chemical recycling of plastics and the development of bioplastics;* Chris Mason, Appleyard Lees Intellectual Property Law, U.K.

**1615 – 1630 T8:** *Bio-based semi-aromatic polyamide electrospun nanofibre membranes;* Xiang Ding, University of Bath, U.K.

**1630 – 1700 IT8:** *Incorporating recycled and recyclable plastics into automotive interiors;* Helena Simmonds, Polestar UK, U.K.

**1700 – 1715 Closing remarks and poster prizes**

# IT1: Exploring cellulose water interactions for making composites

<sup>1</sup>Eichhorn, S.J.

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This talk will present work carried out in our group at Bristol to explore the use of water interactions of cellulose to drive the assembly of composite materials. Initial work, carried out on molecular modelling of cellulose-graphene interactions will show how these materials can ‘bind’ together through the hydrophobic effect.<sup>1</sup> This effect will be explained, and on the basis of entropy, showing how two ‘water hating’ surfaces can ‘adhere’. Furthermore, a full fibril model of cellulose is shown to untwist during molecular modelling simulations, in the presence of water.<sup>2</sup> Following this the work will present the production of cellulose amphiphiles, generated through the octylamine modification of cellulose nanocrystals (CNCs).<sup>3,4</sup> These are high aspect ratio rod-like highly crystalline cellulosic nanomaterials that can be used to reinforce matrices. Herein we will demonstrate their use in forming Pickering emulsions, whereby they sit at the oil-water interface and stabilise the emulsion.<sup>5</sup> We will demonstrate how these emulsions can be used to form a self-healing composite coating<sup>5</sup>, all in the oil-water phase, and how the CNCs can be cross-linked using cystamine to potentially make a reversible and switchable system. Finally, we will demonstrate other uses of cellulose-water interactions in the production of moldable wood<sup>6</sup> and high performance sodium and potassium ion batteries.<sup>7</sup>

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## **IT2: Bio-derived compounds from easily accessed platform molecules**

<sup>1</sup>McElroy, R.

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A bio-derived platform molecule is any compound that can be made from biomass in 3 steps or less in relatively high yield and that contains functionality that can be exploited to add complexity and value. To be viable for use in the expanding bio-economy the feedstocks need to be available at scale and be underutilised. Two such examples are levoglucosenone derived from cellulose and glycidol derived from bio-diesel waste streams.

## **IT3: The intrinsic link between biomaterials and Net Zero**

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Net zero refers to a steady state in which the volume of greenhouse gases entering the atmosphere is balanced by their removal from the atmosphere. Whilst new and cheaper sources of energy are going a long way to reduce Scope 1 and Scope 2 emissions across the chemical manufacturing sector, virgin fossil-based chemicals represent the greatest contribution to a products environmental footprint that cannot be sustainably accounted for by offsetting or carbon capture. Therefore, a new supply chain based upon recycled and biobased building blocks is critically required step on the road towards meeting the Paris Climate Accord. This paper aims to present some of the options, balanced against the challenges and concludes that a paradigm shift is possible, but will not be arrived at easily, or without action.

## IT4: Effect chemicals from waste bio-oils

<sup>I\*</sup>Cole-Hamilton, D. J., <sup>I</sup>Kenyon, P. J., <sup>I</sup>Webb, P. B., <sup>I</sup>Duque Garcia, R., <sup>I</sup>le Goff, R., <sup>I</sup>Furst, M., <sup>II</sup>Mmongoyo, J., <sup>II</sup>Mgaya, J., <sup>I</sup>Julis, J., <sup>I</sup>Bartlett, S., <sup>III</sup>Baader, S., <sup>I</sup>Shi, Y., <sup>II</sup>Mgani, Q.

\*lead presenter

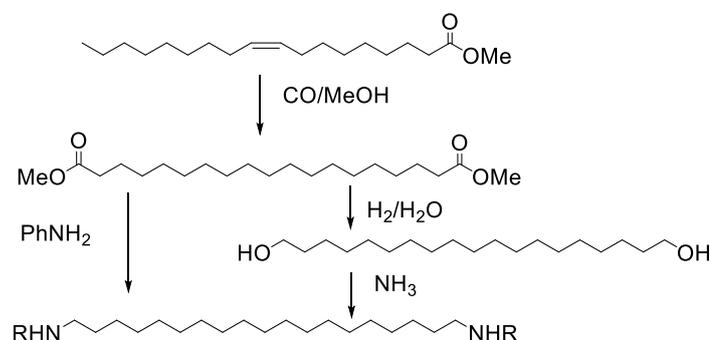
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As oil supplies dwindle and the price increases, it is essential to find new ways of making the many chemicals on which the quality of our lives depends. One approach is to use renewable resources which can be grown. However, there is a tension between using land for fuel or chemicals production and the need to use land to produce food for the rapidly increasing world population. One possible solution is to use waste products for the manufacture of chemicals. In this presentation, we shall discuss the conversion of methyl oleate and oleic acid, a major component of *Tall Oil*, a waste from wood processing, into polymer precursors. We shall also discuss the synthesis of a range of important chemicals from cashew nut shell liquid (CNSL), a waste from cashew nut processing.

We shall show how homogeneous carbonylation,<sup>1, 2</sup> metathesis, and reductive amination<sup>3</sup> can be used to make difunctional esters, acids, alcohols, amines<sup>1, 4-6</sup> for polymer formation<sup>7, 8</sup> from unpurified natural oils containing oleate residues (Figure 1). We shall also describe the formation of *N*-heterocycles by hydrogenation of diesters in the presence of amines.<sup>9</sup>



**Fig 1** Diesters, diols and diamines from methyl oleate.

Cashew nut shell liquid contains interesting phenols *meta* substituted with an unsaturated C<sub>15</sub> chain. We shall describe how it can be used to synthesise tse-tse fly attractants, potentially safe detergents, polymer additives, monomers for polymerisation, large ring macrocyclic lactones and pharmaceuticals.<sup>10-13</sup> These transformations can be carried out using homogeneous catalytic reactions such as isomerising methoxycarbonylation, cross metathesis, isomerising metathesis and hydroxyamination.

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## **IT5: The future of chemistry**

<sup>1</sup>Heslop, A.P.

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Recognizing the urgency to address climate change and reduce environmental impact, BASF is actively driving the adoption of alternative sustainable feedstocks. Leveraging its extensive expertise, the company is investing in research and development to harness the potential of chemical feedstocks derived from renewable sources, such as waste oils and fats. This strategic shift offers numerous advantages, including a significant reduction in greenhouse gas emissions and enhanced resource efficiency.

However, this transition is not without challenges. The chemical industry currently relies heavily on fossil-derived feedstocks, which have established infrastructure and cost advantages. The adoption of non-fossil derived feedstocks requires significant investments in research and development, as well as scaling up production technologies. Additionally, ensuring the availability and affordability of these alternative feedstocks in sufficient quantities remains a concern.

BASF's commitment to sustainability is underscored by its emphasis on collaboration and innovation. The company actively engages in partnerships with suppliers, customers, and research institutions to advance the development and application of non-fossil derived chemicals. By embracing this transformation, BASF aims to create a more sustainable chemical industry.

## **IT6: Catalytic upgrading of polymers – is chemical recycling the answer?**

<sup>1</sup>\*Jones, M.D., <sup>1</sup>Payne, J.

\*lead presenter

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Growing environmental concerns associated with plastic pollution have brought this urgent topic to the mainstream agenda. Whilst renewable and biodegradable polymers have an integral role in mitigating such concerns, it is clear current end-of-life (EoL) options predominantly align with a linear economic model. There is therefore a pressing need to develop alternative and economically viable recycling technologies to align the plastics economy with a circular one. Indeed, comparatively the chemical recycling of polyesters remains vastly unexplored relative to alternative mechanical systems.

The work detailed herein describes a series of simple, well-defined mono- and dimeric zinc complexes and their application for the chemical recycling of a series of polyester and polycarbonate materials. These processes are discussed in the wider context of the literature and future perspectives will be highlighted.

## **IT7: IP trends in the chemical recycling of plastics and the development of bioplastics**

<sup>1</sup>\*Mason, C.J., <sup>1</sup>Barton, A., <sup>1</sup>Jasiewicz, D.

\*lead presenter

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Plastic's myriad of compositions and uses are its strengths. Traditional petrochemical-derived plastics, such as polyolefins, polyesters, polyamides, polyacrylics, polystyrene, and polyvinyl chloride (PVC), have evolved over decades, offering highly-specialised properties for a huge range of applications. They remain highly valuable materials, essential in many areas of modern life, and this will likely continue until greener bioplastic alternatives can sufficiently replicate their performance.

However, continued use is increasingly also likely to be dependent upon such plastics achieving a much higher level of end-of-life recycling as petrochemical-derived plastic waste is a pollutant, taking decades to biodegrade.

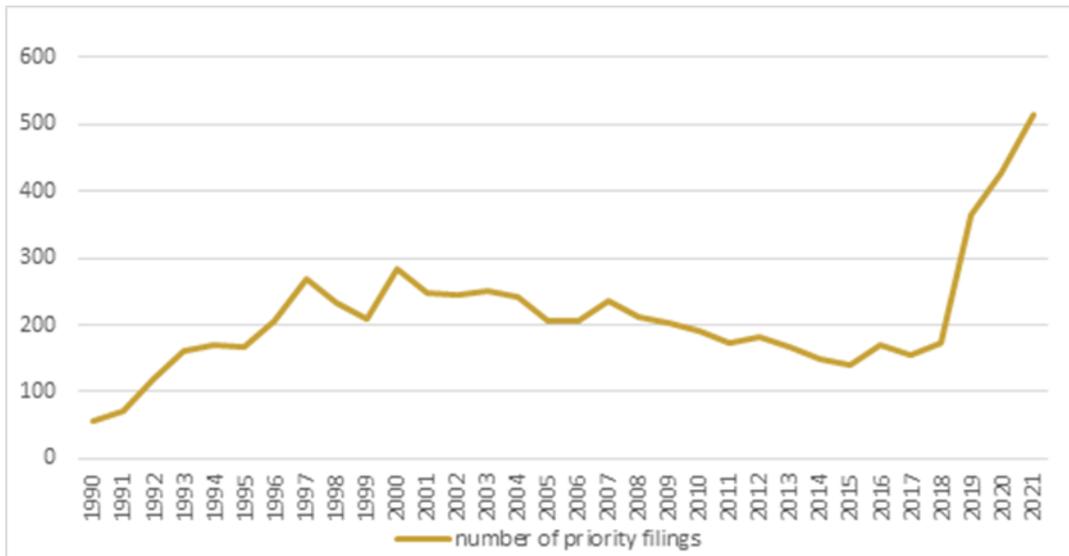
A square metre of landfill filled with waste plastics will include a wide variety of polymers with different chemical compositions, structures and properties. This makes recycling difficult - plastic's myriad of compositions and uses is a weakness when it comes to ease of recycling. A large number of tailored recycling solutions are likely to be needed.

Using patent filing data, we have endeavored to provide a measure of global progress in technologies used to recycle plastic; to gauge where and which recycling methods are taking hold, and the new plastics recycling technologies – or iterations of foundational technology – that are emerging.

We focused on chemical plastic recycling (CR) technologies, including thermal recycling, chemical depolymerisation, and biodegradation. We also looked at downstream innovation toward recovery and modification of the products of these processes.

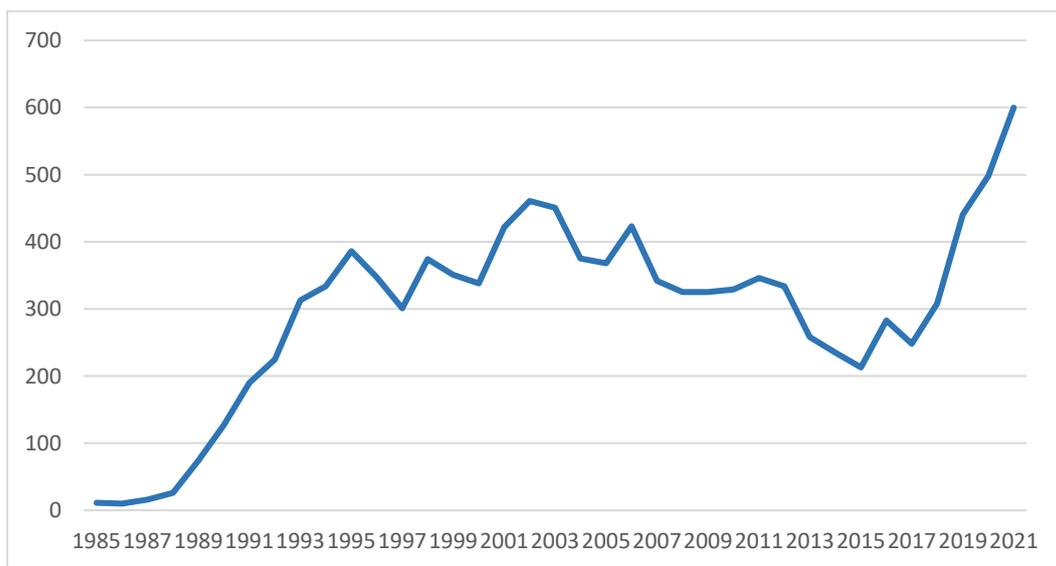
Assuming that innovators want to protect proprietary plastics recycling technology for commercial benefit, making patents a barometer of progress – we do not see innovation developing at equal rates across all types of technologies and territories. Some technology areas are emerging as more technically, and commercially, viable than others. Some territories are taking a strong lead over recent years when it comes to the rate of new technology development.

Broadly, the rate of innovation for plastic recycling has increased markedly in recent years, and a growing number of entities are contributing. Pyrolysis technology is still the main source of innovation, but there is growth in other fledgling technologies including biodegradation and electrolysis.



**Figure 1** – Global patent filing trend for chemical plastic recycling technology over time

We also examined the patent data behind the potential bioplastic replacements for conventional plastics. Here we also found strong recent global growth in new innovations, with a similar trend profile to plastic recycling over recent decades. Application numbers in particular for innovations relating to polylactic acid (PLA), polyhydroxyalkanoates (PHAs), and butylene-based polymers have shown notable recent increases. More broadly, bioplastic innovation is unsurprisingly focused around the two main problems that the industry must solve – providing at least comparable performance to the conventional plastic that it aims to replace, while maintaining its biodegradability credentials (and to add a third – at economical cost!).



**Figure 2** – Global patent filing trend for bioplastic technology over time

Patent activity in these two areas is currently at an all-time high – it remains to be seen whether this recent growth in commercially valuable innovation translates into a real and permanent shift in the plastics industry and the drive toward a more circular economy.

## **IT8: Incorporating recycled and recyclable plastics into automotive interiors**

<sup>1</sup>\*Simmonds, H.C., <sup>1</sup>Holland, R, <sup>1</sup>Tallis, D & <sup>1</sup>Wilson, M.

\*lead presenter

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Polestar is a design-focused electric performance car brand, harnessing refined performance and cutting-edge technology. Our goal is to build sustainable electric cars and to help create a sustainable society. Polestar's Research and Development is based in Coventry UK; here the vehicle's engineering design takes place as well as research for future materials and tech features. Sustainability is a key pillar for Polestar, and we have identified climate, circularity, transparency, and inclusivity as the most important elements of focus for the company. Polymers are widely used across our vehicles, and a significant contributor to its carbon footprint; as such we are committed to reducing the environmental impact of the plastics we use.

Recycling plays an important role for automotive polymers. Recent legislation is putting more demand on manufacturers to use recycled plastics in their vehicles, with a push to closing the loop rather than down-cycling. Polestar are collaborating with academics and recyclers to increase the use of recycled materials in its vehicles and overcome some of the challenges associated with this. We are also aiming to design vehicles so they can be more easily recycled. It is key that the placement of polymers in the vehicle is considered so they can be easily extracted enabling more opportunities to create value from end-of-life vehicles.

Polestar is running a number of live Advanced Engineering projects incorporating recycled and recyclable polymers in automotive interior applications. This includes the ambitious Polestar 0 project. Polestar 0 is our moon-shot aiming to produce a truly climate neutral car by 2030. Polestar plan to share findings from these projects, as well as key challenges still to be overcome. We believe that collaboration is key in ensuring positive change, for this project to be a success we must challenge the status quo and forge a new and better path.

## **T1: Developing a novel ultrasonic biorefinery process and marketable biochemicals**

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Sonichem's award-winning biorefinery process (RSC best enabling technology prize in 2021) sustainably upcycles sawdust, the by-product of forestry, into the biochemicals lignin, microcrystalline and microfibrillar cellulose, and hemicellulose sugars. These carbon-neutral, renewable platform biochemicals have broad applications across multiple sectors including bio-based resins, composites and coatings, cosmetics and personal care. This talk will look at the challenges of developing a scalable process and creating a market for these novel biochemicals.

## T2: Biosensors and biocatalysis for biorefinery

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Linear consumption models maintain our reliance on fossil fuel-based feedstocks and the poor treatment of our waste results in negative impact upon the climate and environment. The use of genetically engineered microbes (GEMs) can provide tractable approaches to address sustainability challenges including the production of energy, chemicals and materials from non-fossil fuel-based sources. Sustainable production of chemicals, materials and energy from renewable biomass and other carbon-rich waste offers one potential alternative to the continued use of finite geological oil reserves. However, in order to compete with current petrochemical refinery processes, alternative biorefinery processes must overcome significant costs and productivity barriers. Pathway design and optimization is a major bottleneck due to the vast number of possible genetic and process variables and the metabolic burden associated with bioproduction. However, genetically encoded biosensors can provide a solution by transducing the target metabolite concentration into detectable signals to provide high-throughput phenotypic read-outs and allow dynamic pathway regulation [1]. In this talk I will present some approaches and activities towards addressing these engineering biology challenges. This will include the development of advanced biorefinery processes by consolidated production of high-value chemicals directly from waste agro-industrial residues [2], microbial processes to degrade and assimilate plastic and other waste feedstocks [3-4], and thirdly the development of underpinning genetic toolbox to control GEMs for sensing, regulation and production [5-7].

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2. Consolidated production of coniferol and other high-value aromatic alcohols directly from lignocellulosic biomass, 2019, *Green Chemistry*, <https://doi.org/10.1039/C9GC02359C>
3. Structural basis of terephthalate recognition by solute binding protein TphC, 2021, *Nature Communications*, <https://doi.org/10.1038/s41467-021-26508-0>
4. Degradation and bioconversion of complex municipal solid waste streams into human biotherapeutics and biopolymers, 2023, *bioRxiv*, <https://doi.org/10.1101/2023.02.13.528311>
5. Development and substrate specificity screening of an in vivo biosensor for the detection of biomass derived aromatic chemical building blocks, 2016, *Chemical Communications*, <https://doi.org/10.1039/C6CC04559F>
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7. Development of High-Performance Whole Cell Biosensors Aided by Statistical Modeling 2020 *ACS Synthetic Biology* <https://doi.org/10.1021/acssynbio.9b00448>

## T3: Building a terpene-based biorefinery

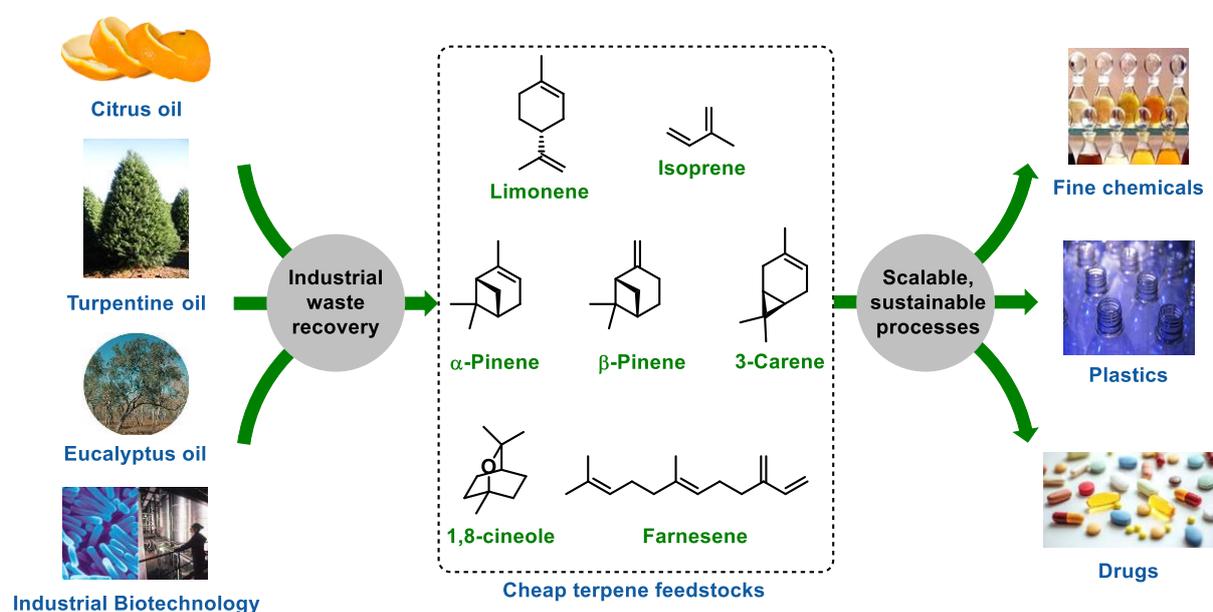
<sup>I</sup>\*Tibbetts, J.D., <sup>II</sup> Bull, S.D.

\*lead presenter

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<sup>II</sup> University of Leicester, U.K.

We have developed a sustainable terpene-based biorefinery model capable of producing multiple valuable chemical products from biorenewable feedstocks sourced from industrial waste streams (e.g., turpentine, waste citrus oils, eucalyptus oils). By using scalable and sustainable chemical transformations, we have been able to produce a variety of bio-derived products including solvents, fragrances, common monomers (e.g. terephthalic acid), a range of terpene epoxides/diols, as well as commonly used drugs such as paracetamol and ibuprofen. This talk introduces the concept of a terpene biorefinery, as well as describing the major terpene feedstocks available, before highlighting ongoing projects into developing our terpene biorefinery model.



**Figure 1:** Terpene-based biorefinery model for the upgrading of industrial waste streams to valuable products.

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3. J. D. Tibbetts, W. B. Cunningham, M. Vezzoli, P. Plucinski and S. D. Bull, *Green Chem.*, 2021, **23**, 5449-5455.
4. J. D. Tibbetts, M. Hutchby, W. B. Cunningham, R. S. L. Chapman, G. Kociok-Köhn, M. G. Davidson and S. D. Bull, *ChemSusChem*, 2023, e202300670.

## **T4: Lignocellulosic biomass conversion into high-value biochemicals**

<sup>I\*</sup>Mora, M., <sup>I</sup>Fàbregas, E., <sup>I</sup>Céspedes, F., <sup>I&II</sup>Puy, N. , S.

\*lead presenter

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<sup>II</sup> Forest Science and Technology Centre of Catalonia, Spain

Given the need in our actual society to substitute the use of fossil fuels, new renewable feedstocks and energy sources are being investigated. Forestry biomass plays a key role in the development of bioeconomy, providing a non-food competitive source of valuable chemicals. In this work, which is encompassed inside the European project LIFE BIOREFORMED, an innovative strategy to produce renewable value-added chemicals and biofuels is developed, using a semi-industrial torrefaction and pyrolysis plant to produce bio-oil and biochar from wood.

Different types of woody biomass were used (Stone pine, Aleppo pine with and without leaves, Oak, Cork oak with bark, Strawberry tree, Heather and Chestnut tree) and compared to produce bioproducts like acids, sugars, antioxidants, phenolic resins, biostimulants and fertilizers. To do so, biomass was processed in a pyrolysis plant, where different operation temperatures were studied (300, 400 and 500 °C) to determine the best conditions for the obtention of the desired products. During this process, two main fractions were obtained, a liquid one (bio-oil) and a solid one (biochar). Bio-oil is a great source for fine chemicals such as sugars (e.g. levoglucosan), acids (mainly acetic acid) and antioxidants like catechol, guaiacol, vanillin and many others. They can be extracted using biorefinery techniques like vacuum distillations, liquid-liquid extractions and column chromatography [1,2]. Good results were especially achieved with biomass coming from pine trees and oak when performing pyrolysis at 400 °C. Acetic acid was obtained with a yield of 15 g/Kg of Aleppo pine and 18 g/Kg of Oak, levoglucosan was obtained with a yield of 10 g/Kg of Aleppo pine and 6 g/Kg of Oak and catechol was obtained with a yield of 3 g/Kg of Aleppo pine and 2 g/Kg of Oak. Moreover, bio-oil was used in the synthesis of phenol-formaldehyde resins, achieving a 70% of phenol substitution, a product currently obtained from petroleum, thus proving more sustainable resins. In this way, bio-oil provided fine chemicals with high-market placing value that have a lot of interest for chemical, pharmaceutical and nutraceutical industries. Biochar, on its own, constituted a readily usable bioproduct itself, used for soil fertilizer applications, water retention, CO<sub>2</sub> capture, biofuels, etc. Furthermore, humic and fulvic acids were extracted from biochar, two very important and widely used commercial biostimulants for plant growth, thereby replacing leonardite, their current fossil-based source.

To conclude, lignocellulosic biomass offers a promising feedstock to produce renewable value-added products, boosting at the same time the management of forests and making a step forward within the context of a circular economy and bioeconomy.

1. M. Mora, E. Fàbregas, F. Céspedes, J. Bartrolí, N. Puy, Production and separation of value-added compounds from pine wood using pyrolysis and biorefinery techniques,

- Fuel Process. Technol. 238 (2022). <https://doi.org/10.1016/j.fuproc.2022.107509>.
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## **T5: Leveraging a green transition with oleochemicals: navigating regulatory landscapes, measuring sustainability, and fostering collaboration**

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In the quest for a sustainable industrial future, the utilization of oleochemicals stands as a compelling solution. This presentation delves into the multifaceted landscape of oleochemicals as a pivotal feedstock for a more sustainable industry. By blending regulatory insights, sustainability metrics, and collaborative efforts, this discussion aims to shed light on the pivotal role that oleochemicals can play in shaping a greener, more responsible future.

Firstly, we will take a deep dive into the value chain of oleochemical products. By understanding this intricate process, attendees will appreciate the complexities and opportunities present in the production and application of oleochemicals. The value chain encompasses cultivation, extraction, refining, and application, and understanding it is critical to making the right choices for a more sustainable industry.

Moving forward, we will examine regulatory frameworks, with a particular focus on the EU deforestation regulation and the Corporate Social Responsibility Directive. By exploring these crucial regulations, we will uncover the pressing need for sustainable alternatives and the essential role that oleochemicals can play in meeting these demands.

Furthermore, we will look at Product Carbon Footprint and Lifecycle Assessment, shedding light on these vital tools for measuring the environmental impact of oleochemical products. These metrics provide invaluable insights into the sustainability of oleochemical feedstocks, aiding both producers and consumers in making informed choices.

Lastly, we will explore the collaborative efforts underway between academia, industry, and end-user applications. This tripartite collaboration is the engine driving innovation in oleochemical products. By bringing together research, innovation, and real-world applications, we can harness the full potential of oleochemicals.

I would be glad to offer valuable insights into the world of oleochemicals and learn how they can be harnessed to navigate regulatory challenges, measure sustainability, and foster collaboration in pursuit of a greener, more responsible industrial future.

## T6: Natural clay catalysts for processing sustainable chemical feedstocks

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Sustainability is now unarguably one of the biggest drivers for innovation within the chemical industry. A key facet of said innovation, is to move away from petrochemical feedstocks. This can be achieved through carbon capture, use of bio-renewables, like fats and oils, and through creating circularity. When switching to these feedstocks the chemical industry also needs to be careful that the processing conditions, for example catalyst technologies, reactor efficiencies, etc., are also sustainable.

At BYK we are looking to catalyst technologies which had fallen out of favour, but are now seeing new opportunities in the future of sustainable chemical feedstocks – particularly natural montmorillonite clay based catalysts. Clays have been used for many years as cost effective strong solid Lewis and Brønsted acid catalysts. The ionising effect of the negatively charged montmorillonite clay surfaces generate Hammett acidities of up to  $-3^1$ , which can be pushed as low as  $-8$  with acid activation. Furthermore, natural montmorillonite clays contain under-coordinated aluminium and iron sites which act as excellent Lewis acids; again with acid treatment the number and potency of the acid sites increases. The potency of the acid sites renders clay catalysts excellent value in oleochemical processing, plastics pyrolysis, Friedel-Crafts alkylation, and/or as off-sets for toxic fluorinated super acids.

This presentation will review the catalytic performance of BYK's clay based FULCAT® catalysts in dimerisation, dehydration, isomerisation, and pyrolysis reactions as well as provide insight in to BYK's ongoing Life Cycle Assessment and sustainability assessment of said catalysts.

1. Theng, B. K. G., (2019), *Clay mineral catalysis of organic reactions*, CRC Press, Taylor & Francis Group, Boca Raton

## **T7: Combining enzyme surface modification and ionic liquids for a facile strategy to enhance biocatalytic degradation of plastics**

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Enzymes can perform many industrially relevant reactions, such as esterification, hydrolysis, oxidation, reduction, and C-C bond formation, with high specificity and under significantly milder conditions than their chemical counterparts. They can perform these reactions on a wide range of substrates, making them highly attractive for many applications. Ionic liquids are highly versatile solvents with tuneable and widely favourable properties such as high thermal stability, negligible vapour pressure, and broad electrochemical windows when compared to conventional solvents. With respect to industrial processing, ionic liquids have advantages in their ability to solvate a large range of substrates, particularly polymers and molecules with otherwise low solubilities in molecular solvents. As a result, research into the use of enzymes as industrial biocatalysts has been gaining ground, particularly in conjunction with ionic liquids. However, enzymes often have very low solubilities in nonaqueous environments, including ionic liquids, and are frequently unstable, limiting the window of usability. Consequently, there is a need to develop new biotechnologies that improve solubility and stability of biocatalysts in ionic liquids to unlock new reactivities of enzymes.

Surface modification of enzymes, to yield solvent-free liquid enzymes, has been demonstrated as a robust method for stabilizing enzymes against temperature, aggregation, and non-aqueous environments. Recent work showed that these new biomaterials are soluble in both hydrophilic and hydrophobic ionic liquids, with enzyme structure preserved in the non-aqueous environment. Using the enzyme glucosidase we were able to demonstrate that in ionic liquids, the optimal temperature for enzyme activity shifted to 110 °C accompanied by activity towards water insoluble cellulose. Solvent-induced promiscuity showed that it was possible to reduce the number of enzymes require for cellulose degradation from 3 to 1. As a result, this nascent technology in conjunction with emerging solvent systems such as ionic liquids could provide a versatile platform for industrial biocatalysis.

Ongoing work now seeks to demonstrate how solvent-free liquid enzymes in conjunction with ionic liquids can be used to broaden the substrate scope for a range of enzymes. Here, we show that ionic liquids can upgrade hydrolysis enzymes for enhanced plastic degradation with a focus on the common polymers PLA, PET, and nylon. Specifically, we demonstrate that surface modification of generic enzymes (e.g. lipases) allows for solubility and stability in ionic liquids such that degradation of plastics to monomers is significantly enhanced through operating at high temperatures (80 – 120 °C) and in solvents capable of softening the otherwise recalcitrant crystalline phases of post-consumer plastic. As such, we provide a blueprint for how any enzyme with plastic degrading capability can be significantly enhanced with relative ease.

## T8: Bio-based semi-aromatic polyamide electrospun nanofibre membranes

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Semi-aromatic polyamides are advanced engineering polymers known for their exceptional thermal and mechanical properties, making them indispensable in high-performance applications. In our previous research, a series of semi-aromatic polyamides have been synthesized based on a renewable monomer, 2,5-furandicarboxylic acid (FDCA). Here, we extended our focus to the development of bio-based semi-aromatic polyamides, specifically poly(hexamethylene furanamide) (PA6F) and poly(decamethylene furanamide) (PA10F). These polymers were electrospun at room temperature, producing nanofibre membranes. In determining the optimal solution, the solution properties such as the solvent system and the concentration of PA6F and PA10F significantly affected the fibre morphology. An increase in polymer concentration leads to a diminution of bead defects, an increase in the nanofibre's diameters, and a decrease in the membrane pore size. The membrane mechanical properties were analysed and correlated to the polymer content and nanostructures. Thermo-gravimetric analysis (TGA) revealed these bio-based semi-aromatic polyamides exhibit thermal stabilities similar to their petroleum-derived counterparts, and the membranes were found to be thermally stable up to 400 °C. These findings provide important guidance for fabricating high-performance semi-aromatic polyamide membranes and expanding their applications.

1. Kamran M, Davidson M G, Tsanaktsis V, et al. *European Polymer Journal*,178 (2022): 111496.
2. Kamran M, Davidson M G, de Vos S, et al. *Polymer Chemistry*, 2022, 13(23): 3433-3443.

## **P1: One-pot chemical recycling of polyethylene furanoate**

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\*lead presenter

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Polyethylene furanoate, or PEF, is a biobased plastic made from FDCA which can be synthesised from biomass. The renewable polymer has been suggested as a renewable alternative to PET in plastic bottles and food containers. The chemical recycling of PET has been intensively studied, but only a few groups have investigated PEF. Our research aims to investigate the complete circular chemical recycling of PEF and to investigate a catalyst for this depolymerisation and repolymerisation.

Gram-scale glycolysis of PEF kinetics was conducted with three catalysts, zinc L-proline, zinc B and zinc acetate, where zinc L-proline and zinc B outperformed zinc acetate. The product of the glycolysis bis(hydroxyethyl)furanoate or BHEF was isolated at 86% yield. In addition to the investigation into depolymerisation, 130 g polymerisation of PEF were conducted using zinc L-proline, titanium citrate, titanium isopropanol and titanium butoxide.

Finally, combining both techniques, a 150 g scale one-pot recycling of PEF was conducted. In this reaction, the PEF was depolymerised to BHEF, then repolymerised back to PEF only using one catalyst at 0.0086 mol%. Due to its activity, even with this lower catalyst loading, the large-scale depolymerisation was conducted in under 5 hours with only a slight excess of ethylene glycol (a ratio of ethylene glycol to PEF of 1:1.2). The product of the repolymerisation was compared to the starting PEF using NMR spectroscopy, SEC, DSC and tensile test and no significant differences were observed. We have found that the one-pot chemical recycling of PEF is possible at lab scales, and highly active catalysts can be used for both depolymerisation and repolymerisation. This chemical recycling process did not impact molecular weight, thermal properties or mechanical properties. Before we can replace fossil fuel-based plastics, we need to have a strategy for the end-of-life of their replacements. Depolymerisation might be one of the solutions.

## **P2: Eco-sustainable synthesis of $\alpha$ -hydroxylated fatty acids: an opportunity for the valorisation of waste wool grease**

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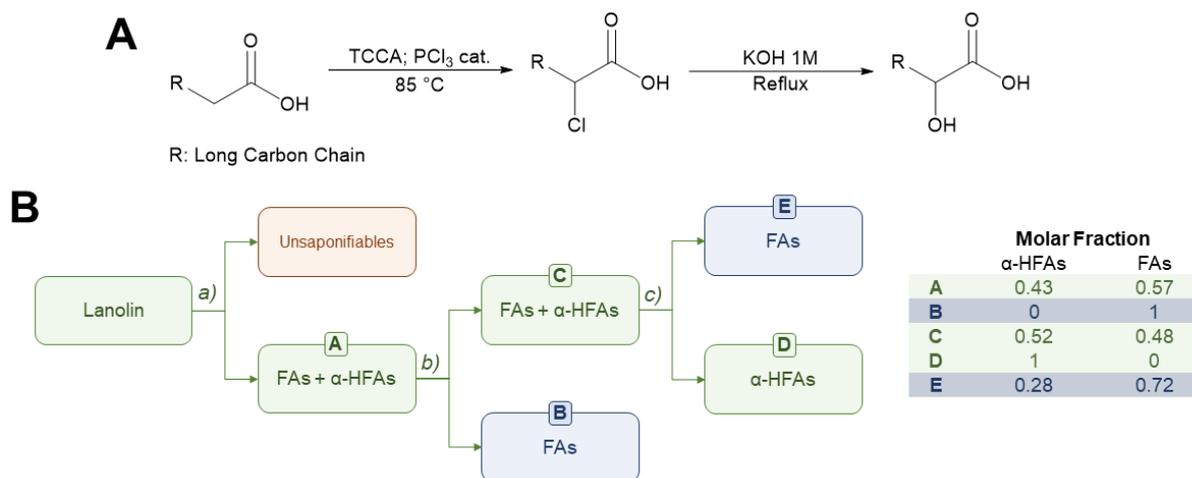
\*lead presenter

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Fat biomasses represents a significant portion of food waste, often not valorised and disposed of with systems that are harmful to the environment <sup>1</sup>. Among these, lanolin, grease deriving from sheep wool scouring, could represent a renewable waste biomass, unique in properly said fatty acids (FAs) and, above all, alpha-hydroxy fatty acids ( $\alpha$ -HFAs) richness.  $\alpha$ -HFAs can be used in various production fields (cosmetics, pharmaceuticals, food) due to their chemical-physical and biological properties, however their employment is limited by poor availability and high cost. Therefore, a possible valorisation of FAs is represented by their conversion into  $\alpha$ -HFAs.

The synthesis of  $\alpha$ -HFAs is traditionally carried out in two steps:  $\alpha$ -halogenation and replacement of the halogen with a hydroxyl group. Halogenation is carried out using organohalogens or diatomic halogen itself, both toxic and dangerous, and non-eco-sustainable solvents. As an alternative, it is here proposed the use of trichloroisocyanuric acid (TCCA), economical and harmless, as a halogenating agent in a solvent-free reaction (Figure 1A). With the use of TCCA (1.4 eq.) and a catalytic quantity of  $\text{PCl}_3$  (0.3 eq.) it was possible to obtain a complete conversion of three individual medium-long chain fatty acids (myristic, palmitic and stearic) and also of their mixture in the respective  $\alpha$ -chlorinated derivatives in 24 h at 85 °C, the temperature at which the substrates are in the molten state. The  $\alpha$ -chlorinated acids were then converted into  $\alpha$ -HFAs by treatment with KOH 1 M for 24 h at reflux (65% yield) <sup>2</sup>.

In order to prove the feasibility of this procedure, acid components of lanolin were recovered by saponification with KOH; FAs were separated from  $\alpha$ -HFAs benefitting of the different solubilities in organic solvents, namely methanol and cyclohexane (Figure 1B). Composition of the different portions (A-E) were assessed through <sup>1</sup>H-NMR and GC-MS <sup>3</sup>. After that, fractions B and E were thoroughly mixed and subjected to alpha-hydroxylation, with only slight differences and changes.



**Figure 1A:** Reaction scheme for alpha-hydroxylation of fatty acids.

**Figure 1B:** Schematic representation of lanolin acid components fractioning, along with molar fraction composition. *a)* KOH 10% (w/v), reflux, 48h; *b)* Methanol, rt, 2h; *c)* Cyclohexane, rt, o.n.

1. R. Sawangkeaw and S. Ngamprasertsith, *Renewable and Sustainable Energy Reviews*, 2013, **25**, 97–108.
2. V. Bertolini et al., *ACS Omega*, 2021, **6**, 31901–31906.
3. C. Morano et al., *Molecules*, 2023, **28**(4), 1635.

### **P3: The policies driving chemicals industry defossilisation and their potential role in Switzerland**

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Today **fossil oil and gas continue to dominate** the global supply of energy and raw materials used for **product manufacturing** which uses approximately 15% of global oil and 9% of gas demand (a total of 730 Mt/year of fossil carbon). Some of this carbon is emitted during production, the rest becomes part of the molecules and downstream products. Because these products contain carbon, virgin fossil carbon would need to be **replaced with carbon** from **CO<sub>2</sub> captured** from the atmosphere (directly or from biogenic point source emissions or via the use of biomass) and/or recycled carbon to defossilise these products. The **European Union (EU)** and the **United States (US)** are two of the largest markets for sustainable products and have some of the most developed policy portfolios driving **defossilisation**. Defossilisation encompasses the decarbonisation of energy inputs and a reduced reliance on fossil resources by recycling fossil carbon and decreasing the amount of fossil carbon in products by replacing it with carbon from the atmosphere.

**Policy plays a crucial part** in driving the uptake of **new technologies** and **solutions** as they mature and become competitive with the conventional fossil resources. Policymakers have largely focused on reducing emissions from power and fuels because these have a larger contribution to global emissions (31.5 bn tCO<sub>2</sub>/year) but are increasingly addressing emissions of the wider economy. This includes chemicals and manufactured products, addressing the emissions from the processes that produce them and the end-of-life of the products. **The report (available at [www.cloop.ch/literature](http://www.cloop.ch/literature))** analyses policies in these jurisdictions providing an assessment on their impact on the chemicals and product manufacturing industries in terms of strength, reach, focus and clarity. There is **no overarching policy framework for defossilisation**, and most policies reviewed are focused on decarbonisation and some of these become indirect drivers for defossilisation.

The strongest levers currently driving defossilisation are **policy measures that promote the uptake of non-fossil and recycled feedstock**. These measures include policies that **directly target or incentivise the uptake** of non-fossil virgin feedstock (e.g. incentives for non-fossil and recycled feedstocks, green finance and RD&D funding programmes such as Horizon Europe) and policies that **indirectly induce use** of recycled fossil feedstock and atmospheric carbon (e.g. emerging policy proposals related to of Carbon Capture & Utilisation). In the EU, the proposed inclusion of Carbon Capture & Utilisation (CCU) in the EU Emissions Trading System (ETS) combined with the renewable hydrogen mandate for the EU industry (42% by 2030 and 60% by 2035) are expected to be a driver for defossilisation when implemented, but both are uncertain. In the US, the 45Q tax credit and Hydrogen Production Tax Credit could offer support to use captured CO<sub>2</sub> and production of low carbon hydrogen in the US, although hydrogen may be directed to fuel use. Furthermore, funding programmes can be a key mechanism in supporting research and commercialisation of new technologies. The EU and US

have introduced different research and development funding mechanisms, which have been used to deploy innovative and more sustainable technologies.

**Policy measures that increase the cost of carbon emissions and/or the use of fossil feedstock** by industry are also popular approaches amongst policy makers to reduce GHG emissions. They do not prescribe technologies, thereby allowing industry to determine the most efficient way to reduce emissions. Carbon pricing, fees on fossil feedstock use or decreasing subsidies for fossil carbon implicitly support the use of non-fossil and recycled feedstocks where raw materials are used both for energy and feedstocks (e.g. steam cracking), and where there are synergies between raw materials and fuel supply chains (e.g. the use of waste biomass for energy in ethanol production plants alongside bio-based feedstocks). The EU's Carbon Border Adjustment Mechanism (CBAM) could provide a strong driver for defossilising energy inputs, and thereby feedstocks where raw material inputs have dual uses. The CBAM is an EU policy but would influence both EU and global producers that export to the EU.

**Policies driving the transition to a more circular economy** have focused on recycling of conventional plastics. These have included targets on the amount of recycled content in products, bans on specific single use plastic items, taxes on the use of virgin fossil-based plastics and extended responsibility for collection and recycling for producers. Policies around the circular bioeconomy related to bio-based plastics and to the circularity of other chemicals and their derivatives are currently limited, but recent proposals suggest that policymakers are paying increasing attention to bio-based solutions to promote a more circular economy.

**Policy measures promoting the demand** for chemicals from non-fossil and recycled feedstocks include green labelling and design requirements and green public procurement. However, their strength is limited by being voluntary (green labels) and being limited to a niche segment of the market (public procurement). Green public procurement policy may have a more significant impact for pharmaceuticals, compared to chemicals, due to the higher share of healthcare spending in Government expenditures.

This report was funded by F. Hoffmann-La Roche AG and commissioned by cloop, a Swiss association, which has recently been established to accelerate the development of defossilisation solutions in Switzerland. This report raised some key questions for the defossilisation of the Swiss industry:

- What is the impact of EU and US policies on where investment in defossilisation will take place? For example, will renewable hydrogen roll out from constrained electrolyser manufacturing be focused on the US due to the tax credits available under the Inflation Reduction Act?
- Should Switzerland develop similar policies as the EU and US to promote investment in defossilisation?
- What opportunities are there for “friend-shoring” to defossilise industry in Switzerland? i.e., manufacturing and sourcing from countries with shared values, thus leading to energy and resource security?
- Which technical solutions will be the most cost competitive and where are they likely to be first located, considering renewable or recycled carbon and other resources, as well as policy?
- Which Swiss companies and technology developers could develop and deploy technology to provide renewable and recycled feedstocks, and where? What support do they need?

## P4: Carbon dioxide utilization in block polymers: catalysis and functional materials

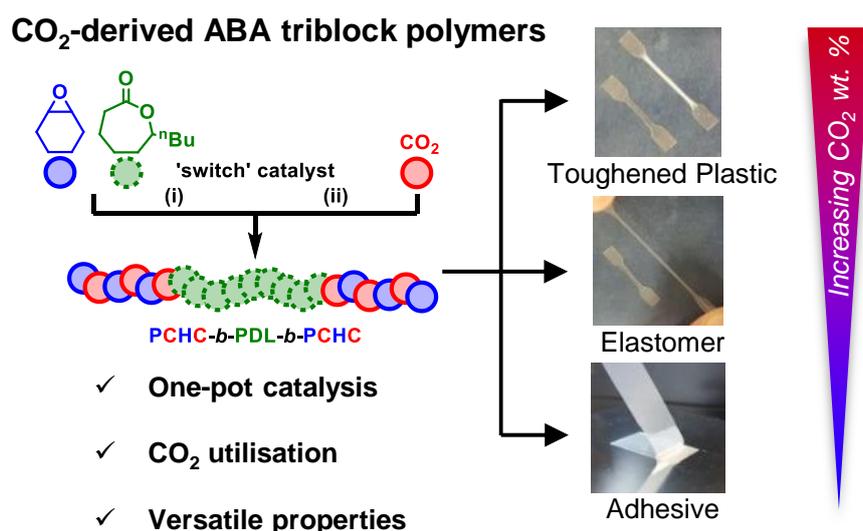
<sup>I\*</sup>Sulley, G.S., <sup>I</sup>Gregory, G.L., <sup>I</sup>Chen T.T.D., <sup>I</sup>Carrodeguas, L.P., <sup>I</sup>Trott, G.,  
<sup>II</sup>Santmarti, A., <sup>II</sup>Lee, K-Y., <sup>III</sup>Terrill, N.J., <sup>I</sup>Williams, C.K.

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A drive towards a more sustainable plastics future is a strong focus of academic research within polymer science and technology. Polymerization catalysis can afford routes to block copolymers from a mixed monomer feedstock, with the potential to utilize renewable resources. Some catalysts are now able to directly incorporate carbon dioxide into polymers, by copolymerization with epoxides, which provides a useful strategy for the utilization of this renewable C<sub>1</sub> source. This presentation will focus on the synthesis of ABA-type poly(carbonate-*b*-ester-*b*-carbonate) triblock polymers, with precise CO<sub>2</sub> incorporation into the polymer backbone. The polymers are prepared using a new organometallic Zn(II)/Mg(II) heterodinuclear catalyst. The catalyst shows high selectivity (>99%) for CO<sub>2</sub> uptake, enables near quantitative conversion of monomers, and facilitates excellent end-group control to form hydroxyl-telechelic block polymers with molar masses ranging between 38–71 kg/mol. The polymers exhibit microphase separation of the constituent blocks, as determined by thermal and mechanical analysis, as well as showing reasonable thermal stability to degradation ( $T_{d,5}$  ~280 °C). The material properties are tuned by controlling the monomer feed ratio, which enables accurate control over polymer composition and of CO<sub>2</sub> content. The resulting polymers are toughened plastics (15 wt% CO<sub>2</sub>), elastomers (8 wt% CO<sub>2</sub>), and pressure-sensitive adhesives (6 wt% CO<sub>2</sub>).

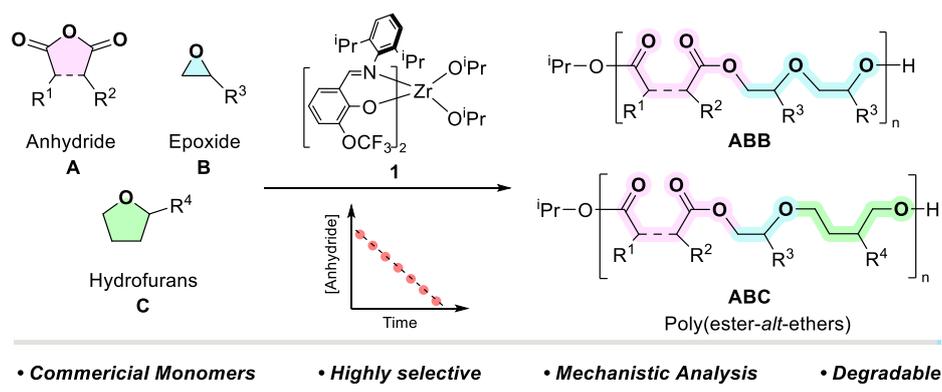
## P5: The synthesis, mechanistic and property evaluation of poly(ester-*alt*-ethers) from commercial monomers and a Zr(IV) catalyst

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\* lead presenter

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Polyesters are seen as sustainable alternatives to complement and replace current petrochemical-derived, commodity polymers.<sup>1</sup> One method to synthesize polyesters is through the catalytic ring-opening copolymerization (ROCOP) of anhydrides (**A**) and epoxides (**B**) using Lewis acidic metal complexes.<sup>2</sup> The products typically exhibit alternating **AB** monomer sequencing and the monomers for this process are numerous, commercial and frequently accessible from bio-based sources. Poly(ester-*alt*-ethers), an important subclass of polyesters, combine the inherent flexibility of ether linkages with the characteristic degradability of esters. Currently, their synthesis requires either the use of bespoke monomers,<sup>3</sup> or under-explored synthetic protocols.<sup>4</sup>

In this work, a novel Zr(IV) catalyst, **1**, bearing phenoxyimine ligands and isopropoxide co-ligands for the co-polymerization of anhydrides (**A**), epoxides/oxetane (**B**) and tetrahydrofurans (**C**) is described.<sup>5</sup> The catalyst operates with excellent control to yield unusual -**ABB**- and -**ABC**- type polymers giving a straightforward means to moderate the chain-length between ester linkages. Kinetic analysis reveals a second order rate-law, 1<sup>st</sup> order in catalyst and epoxide and zero order in anhydride and THF. The new colorless **ABB/ABC** polymers exhibit lower glass transition temperatures and increased ester hydrolysis degradation rates compared to their analogous **AB** counterparts, consistent with greater backbone flexibility.

The new Zr(IV) catalyst for cyclic ether and anhydride ROCOP combines good rates, unusual selectivity, and high polymerization control to yield poly(ester-*alt*-ethers). The catalysis utilizes commercially available monomers, such as phthalic anhydride, butylene oxide/oxetane, and tetrahydrofurans. The polymerization kinetics and reactivity studies underpin a new type of **ABB/ABC** sequence control and polymerization mechanism. These amorphous, “soft” polymers are relevant in phase separated block polymer structures, e.g., to make thermoplastic

elastomers or plastomers. In the biomedical context, these polymers could represent degradable alternatives to widely used polyethers.

1. Y. Zhu, C. Romain, C. K. Williams, *Nature*, **2016**, *540*, 354
2. A. J. Plajer, C. K. Williams, *Angew. Chem. Int. Ed.* **2021**, *61*, e202104495.
3. J. M. Raquez, P. Degée, R. Narayen, P. Dubois, *Macromolecules*, **2001**, *34*, 8419.
4. H. L. Hsieh, *J. Macromol. Sci. A* **1973**, *7*, 1525.
5. R. W. F. Kerr, C. K. Williams, *J. Am. Chem. Soc.*, **2022**, *144*, 6882.

## **P6: Sustainable olefin production in the Teesside**

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\*lead presenter

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To achieve the goal of a 45% reduction in greenhouse gas emissions by 2030 and ultimately reach net zero by 2050, active measures are required to replace fossil fuels with more renewable resources. The chemical industry is heavily reliant on natural gas for energy and feedstocks. One of such feedstocks widely produced and used in the sector is olefins. Olefins, particularly ethylene, is a major building block for the production of a wide range of chemical products, including pharmaceuticals, polymers and surfactants. Ethylene is typically produced from the steam cracking of naphtha or natural gas, contributing to greenhouse gas emissions globally. Identifying and using alternatives to fossil-based feedstocks for ethylene production will have a significant positive impact on the goal towards net zero. The Teesside region houses one of Europe's largest clusters of chemical and process industries. From bioethanol and polymers to vaccines and jet fuels, the Teesside industry cluster produces a wide range of products that can be linked to olefins. Here, an Innovate UK-funded project aimed at sustainable olefins production in the Teesside is presented. The goal of the project is to identify viable feedstocks, technologies and supply chains for sustainable olefins production in the Teesside. This project aims to develop a strategic roadmap for waste valorisation and industrial symbiosis within the region.

An initial mapping of the input and output streams in the region showed multiple CO<sub>2</sub> emission points as well as biological and chemical wastes. Some industries are capturing and purifying some of the CO<sub>2</sub> streams for reuse or as products used within and outside of the cluster. CO<sub>2</sub> is a well-researched feedstock option for sustainable ethylene production; hence it is under consideration for use for ethylene production in the region. Furthermore, bioethanol is being considered as a feedstock option in this project. Bioethanol is produced in the Teesside cluster as a co-product of the production of high-protein animal feed. It is a potentially viable option for sustainable ethylene production depending on the outcome of economic and environmental impact analyses. Lastly, this project will also consider waste plastics as a potential feedstock. In the region, a few companies produce and/or recycle plastics. Some plastics also end up in landfills. The goal is to identify viable waste plastic streams that could be converted to ethylene. Relevant technologies such as the CO<sub>2</sub> to methanol to ethylene route for CO<sub>2</sub> conversion, ethanol dehydration and plastic pyrolysis are being explored. Supply chain implications, economic viability and environmental impact assessments will also be carried out. The outcome of this project will provide relevant information that would enhance a circular chemical economy in the region and ultimately, industrial symbiosis within the region.

In the poster, an introduction of the North East Process Industry Cluster (NEPIC), the organisation taking the lead on this project will be provided. The Teesside industry cluster will be described, and a map of the industry waste streams will be presented. The scope of this project will be summarised, including the initial findings.

## P7: Al(III)/ M(I) Catalysts for High Rate Epoxide and Anhydride Ring Opening Copolymerisation and High Molar Mass Polyesters.

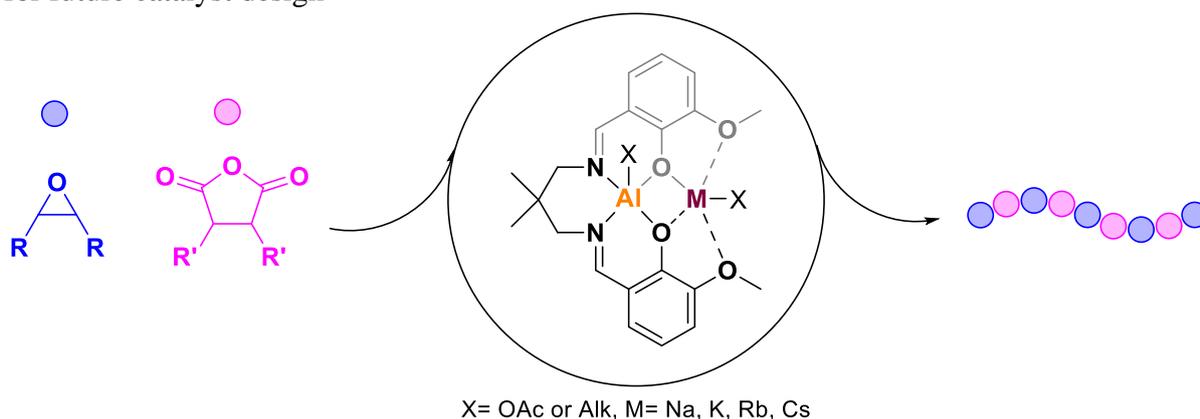
<sup>I\*</sup>Concilio, M., <sup>I</sup>Diment, W.T., <sup>I</sup>Gregory, G.L., <sup>I</sup>Kerr, R.W.F., <sup>I</sup>Phanopoulos, A.,  
<sup>II</sup>Buchard, A., <sup>I</sup>Williams, C.K.

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The precise synthesis of polyesters through epoxide/anhydride ring-opening copolymerization (ROCOP) represents a versatile, atom-efficient method for producing sustainable polymers. To be effective in applications such as plastics, elastomers, and fibers, efficient and selective polymerization methods that yield predictable, high molecular weight polyesters are required. Current catalysts, however, often suffer from low activity and cannot tolerate low catalyst loadings. In this study, we present a series of innovative heterodinuclear complexes, featuring combinations of Al(III)/M(I) (where M = Na, K, Rb, Cs). These complexes exhibit exceptional activity, tolerance to low catalyst loadings, and perfect polyester selectivity. Particularly, the organometallic heterodinuclear Al(III)/K(I) complex, when used with a diol co-initiator, is tolerant to various epoxides/phthalic anhydride combinations, generating high molecular weight ( $M_n$  up to  $91 \text{ kg mol}^{-1}$ ), monodisperse polyesters ( $D = 1.05 - 1.10$ ) with precisely defined hydroxyl chain-ends. Moreover, this catalytic system enables the synthesis of triblock polyesters through switchable catalysis with monomers such as phthalic anhydride, vinyl cyclohexene oxide and  $\epsilon$ -decalactone. These results evidence the remarkable efficiency of these heterobimetallic complexes in ROCOP of epoxides and anhydrides, offering valuable insights for future catalyst design



TOF >  $1000 \text{ h}^{-1}$  (0.025mol% vs. anhydride, 100 °C)  
>99% Polyester Selectivity  
High Molar Mass Polymers  
Synergic Metal Combination

## P8: Development of ZnInS Nanoparticles for the Photocatalytic Conversion of Methanol to Ethylene Glycol

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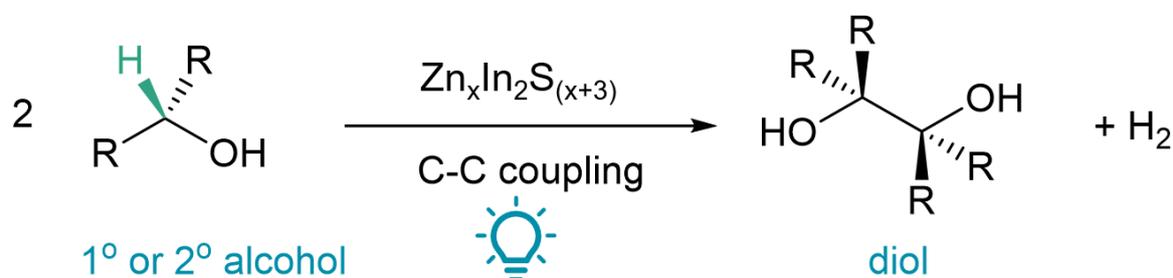
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**Keywords:** heterogeneous photochemistry, semiconductor nanomaterials, ethylene glycol

Current industrial methods for the production of ethylene glycol (EG) use chemicals from petroleum sources, require large amounts of water, can be unselective, and need energy-intensive separation processes to isolate the EG product.<sup>1</sup> Previous literature work has shown that EG can be directly synthesised from methanol *via*  $\alpha$  C-H activation, using semiconductor nanoparticles, such as zinc indium sulfide ( $\text{Zn}_x\text{In}_2\text{S}_{(x+3)}$ ), as a heterogeneous photocatalyst.<sup>2</sup> This promising work showed a difference in selectivity for ethylene glycol when the composition of zinc indium sulfide is varied.



**Scheme 1 - Methanol to ethylene glycol transformation, with zinc indium sulfide as a heterogeneous photocatalyst**

In the earlier work,  $\text{ZnIn}_2\text{S}_4$  was reported to be an inactive photocatalyst for EG formation from methanol, despite having very similar photophysical properties to  $\text{Zn}_2\text{In}_2\text{S}_5$ , which was reported to be active for this reaction. In this work, we revisited this claim by synthesising  $\text{ZnIn}_2\text{S}_4$  using a rapid hot injection technique. We were able to show that this material is, indeed, active for the transformation of methanol to EG. The effect of the light source, co-catalyst and other additives on the photoactivity and selectivity of the process will also be presented.

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## **P9: Valorisation of waste polyolefin plastics using Lewis acidic ionic liquids**

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Waste polyalphaolefin plastics, such as polyethylene and polypropylene, can undergo pyrolysis to yield a mixture of alphaolefins and paraffins. While this method has been utilized for transforming discarded plastics into diesel fuels, it poses significant economic and environmental considerations. An alternative approach involves the conversion of waste polyalphaolefin plastics into paraffin waxes, a value-added product, along with a naphtha fraction rich in 1-olefins. This project focuses on the conversion of 1-olefins in the naphtha fraction into lubricating base oil, using borenium ionic liquids and liquid coordination complexes (LCCs). This dual-product strategy enhances the economic viability of the entire process.

Our research team has previously shown that borenium Lewis acidic ionic liquids [1] and liquid coordination complexes (LCCs) [2] are effective substitutes for  $\text{BF}_3$  in the catalytic oligomerization of 1-decene, resulting in the production of lubricating base oil with properties matching those of industrial base oil. However, when employing waste polyolefins plastic as the feedstock, the distinct fraction distributions present a challenge due to the competing reactions which are specific to reaction conditions. This application requires a robust catalyst and the use of cheap and available materials. Addressing these challenges will be essential for the continued development and optimization of this process for sustainable and economically viable waste polyolefin plastic recycling.

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## P10: Utilization of a ligno-cellulose material for rifampicin adsorption

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There is an increased burden of different toxic pollutants in various water bodies which have been termed emerging contaminants<sup>1</sup>. The impact of these emerging contaminants is a threat to human health<sup>2</sup>. It is essential to develop an eco-friendly and renewable material for the removal of these pollutants and the promotion of environmental sustainability. Ligno-cellulosic materials are abundant, renewable, and biocompatible, making them potential candidates for water treatment because of their good mechanical stability, easy modification and biodegradation<sup>2</sup>. The aim of this study is to investigate the adsorption capacity of acid modified sawdust in the removal of the antibiotic rifampicin from its aqueous solutions. Rifampicin was used in this study due to *Mycobacterium tuberculosis* rifampicin resistance<sup>3</sup>. The sawdust was blended, sieved, and washed to produce a material with different particle sizes varying from 90 to 850  $\mu\text{m}$ . In this study, a size range of 180-250  $\mu\text{m}$  was selected for both untreated and acid-treated sawdust. Sawdust was treated by mixing it with 2M sulphuric acid for 24 hours and washing several times with water to achieve neutral pH levels of the washings. For this study, the pH of the rifampicin solution, its initial concentration, contact time and temperature of the batch adsorption of rifampicin were investigated on untreated and treated sawdust. Also, the characteristics such as zeta potential, particle size distribution and the pH point zero charge ( $\text{pH}_{\text{pzc}}$ ) were determined in the present study. Using a 25  $\mu\text{g}/\text{ml}$  solution of rifampicin, at the pH 3, the higher level of the antibiotic adsorption (73.00%) was achieved by applying the treated sawdust as opposed to the adsorption on the untreated sawdust (62.60%). As the solution pH increased to 7, the corresponding removal efficiencies were reduced to 52.45% for the treated sawdust and to 32.79% for the untreated adsorbent. Also, the rifampicin adsorption levels from the solution kept at 35°C, were higher for the treated sawdust, 55.60%, as compared to 34.62% for the untreated sawdust. The 48 hrs of the contact time between the particles of the sawdust and the antibiotic solution resulted in the 57.2% removal efficiency on the treated sawdust, compared to 46.29% on the raw sawdust. The treated sawdust had a slightly lower negative zeta potential -3.82 mV than the raw sawdust -3.63 mV. This could be attributed to the chemical treatment process which could have influenced the adsorption capacity of the treated sawdust. The attributes of the lignocellulose material from sawdust, determined in this study, are the pre-requisites of an efficient adsorbent suitable for the removal of rifampicin from wastewaters.

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## **P11: Chemical recycling polypropylene using a novel nickel sulphide catalysts.**

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Global production and consumption of plastic has grown exponentially due to its ubiquitous nature in products that range from packaging and textiles to medical equipment and household goods [1]. With this increasing global plastic production there has been an accumulation of plastic wastes in the environment and in 2015, approximately 6300 Mt of plastic waste had been generated globally. However only 9% had been recycled, 12% was incinerated, and 79% was accumulated in landfills or the natural environment. If the current production and waste management trends continue, about 12,000 Mt of plastic waste will be in landfills or in the natural environment by 2050 [2-4]. This accumulation of plastic waste in the environment requires a route of transformation into a valuable resource to close the loop and establish a plastic circular economy if we are to achieve the Net Zero target by 2050. Hydrocracking, which is a promising alternative to pyrolysis of plastic waste with the use of a bifunctional catalyst, provides a platform to transform plastic waste into useful chemical feedstocks. Here the acidic function is provided by an acidic support such as zeolites for cracking and hydrogen transfer provided by hydrogenating metals such as platinum and palladium [5]. Due to the high cost and scarcity of noble metals, nickel has been targeted as a substitute metal.

Sulfided nickel, an established hydrocracking and hydrotreating catalyst for hydrocarbon refining, was synthesized on zeolite support for the hydrocracking of polypropylene. Zeolite Beta was impregnated with the single-source precursor (SSP) nickel (II) ethyl xanthate using 5 wt.% Ni loading. Non-sulfided Ni (5 %) and 1% Pt loading on zeolite beta supports were also synthesized using wet impregnation from Ni and Pt precursors and used to compare with the sulfided nickel catalysts. All catalyst supports were dried at room temperature and calcined in static air at 500 °C (2 °C/min) for 5 h. Prior to hydrocracking, the impregnated catalysts were reduced in H<sub>2</sub> or He flow (50 cm<sup>3</sup> min<sup>-1</sup>) at 380 and 480 (10 °C min<sup>-1</sup>) for 6 hrs and characterised using N<sub>2</sub> adsorption. Polymer hydrocracking was carried out in a stainless-steel Parr anchor stirrer batch reactor (300mL) where the activated catalyst was mixed with polymer pellets in a 10: 1 ratio. All reactions were carried out at 330 °C, for 60 minutes with a starting pressure of H<sub>2</sub> (20 barg) [5].

From the results, SSP-derived 5wt%Ni@Beta yielded a 95 wt.% conversion of a polypropylene feed. Liquid and gas products were quantitatively analysed by gas chromatography–flame ionization detection (GC-FID) and gas chromatography–mass spectrometry (GC-MS), revealing a strong selectivity to saturated hydrocarbons. The gas product distribution was between C<sub>1</sub>-C<sub>7</sub> and Pt-Beta gave a balanced product of propane (C<sub>3</sub>) and iso-butane (i-C<sub>4</sub>), with an i-C<sub>4</sub>/nC<sub>4</sub> ratio = 2.5. The unsulfided Ni-Beta, gave a high yield of methane (C<sub>1</sub>). Due to the diversity of polymers, additives and other types of waste that could contaminate even relatively pure polyolefin waste streams, this is an important consideration for advancing the technology readiness level of any chemical recycling technology for polymers beyond uncatalyzed pyrolysis

Keywords: Polypropylene, zeolite beta, plastic waste, SSP-Nickel, hydrocracking

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## **P12: Sawdust: a sustainable material for the removal of antibiotics dissolved in water**

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The presence of antibiotic residues in the environment has led to the spread of antibiotic resistance, which is a global threat to human health<sup>1</sup>. Major sources of these pollutants in waterbodies are untreated sewage, effluents from wastewater treatment plants and agricultural run-off<sup>2</sup>. Simultaneously, the sustained global population growth increases the demand for natural resources like wood, industrial processing of which also generates more waste materials<sup>3</sup>. This study focuses on applying such a waste product, – sawdust from Mahogany (*Swietenia mahagoni*) wood, in water treatment for the removal of the antibiotic vancomycin. The World Health Organisation has classified vancomycin as being at risk of losing therapeutic efficacy due to increased resistance by priority pathogens such as *Enterococcus faecium*<sup>4</sup>. Minimising the vancomycin discharge into the environment would help to contain this rise in resistance.

The sawdust was sourced from mahogany trees (Lagos, Nigeria). After washing, drying, and grinding to a particle size between 38 to 850  $\mu\text{m}$  a subsample underwent a pre-treatment with 30% w/v sulfuric acid. Adsorption experiments were conducted with vancomycin hydrochloride dissolved in water at a concentration of 10  $\mu\text{g/mL}$ . Quantitative analysis involved an HPLC instrument fitted with a photodiode array detector.

Material properties were characterized using Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM). SEM images showed that the materials were rod-like in shape with an average particle size of  $8.003 \pm 5.610 \mu\text{m}$ , and  $4.124 \pm 1.209 \mu\text{m}$  for both the untreated and treated sawdust, respectively. The zeta potential values of both the untreated and treated mahogany sawdust particles were  $-14 \pm 1.2 \text{ mV}$  and  $-20.4 \pm 2.12 \text{ mV}$  respectively, indicating negative surface charges for both adsorbents. The increase in the absolute value of the zeta potential after acid treatment is a likely consequence of breaking intermolecular bonds which would expose more negatively charged functional groups on the sawdust surface. In adsorption studies untreated mahogany sawdust reduced the concentration of vancomycin in water by more than 40% within 5 minutes of contact time between adsorbent and antibiotic solution. The optimal contact time for the removal of vancomycin was found to be 30 minutes for untreated sawdust, and 10 minutes for the treated sawdust. Quicker vancomycin adsorption by acid treated sawdust can be explained by the evidenced reduction in sawdust particle size and the increased availability of functional groups on the adsorbent surface. These studies provide experimental evidence, that waste material from Mahogany

wood processing was an effective adsorbent of the antibiotic vancomycin in water treatment, and that its adsorption efficacy can be further enhanced by acid treatment.

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## **P13: Realizing more economically competitive PLA through improved lactic acid isolation and lactide synthesis**

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Poly(lactic acid) (PLA) is the world's most consumed bioplastic, a material which is crucial to achieving a circular economy. However, it currently has a few main limitations hindering it from replacing traditional polyolefins. The main being PLA's synthetic route is economically challenging with multiple energy-intensive/poorly optimised steps, making it expensive compared to non-degradable materials. This is especially for the synthesis of lactide – the monomer precursor used to make the polymer. Our group is working with iCAST (Innovation Centre for Applied Sustainable Technologies) and industry partners to develop novel heterogeneous catalyst systems for the synthesis of lactide monomer from biomass sources (sugar/cellulose). So far we have studied various heterogeneous catalysts for the transformation of cellulosic waste to lactide and have come across a promising method to isolate pure lactic acid from dilute aqueous solutions. This novel technique provides a potential scaffold to improve the economics and isolated yield of lactic acid fermentation while reducing waste. Combined with improved catalytic systems we hope this project will lead to tangible impacts on PLA manufacture at scale.

## **P14: New RAFT polymers, synthesis and kinetics, derived from plant oils**

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Plant oils are an abundant renewable resource that have been demonstrated in the literature to be a suitable feedstock for polymers with interesting properties (low T<sub>g</sub>, hydrophobicity, functionalisation of unsaturations in pendant groups). In this work plant oil-based monomers (POBMs) were synthesised from four different feedstocks via a one-step, industrially relevant reaction, and the kinetics of their polymerisation in a RAFT system were investigated. The reactions of the feedstock oils have been investigated in terms of the average chain length of fatty acids; the degree of unsaturation of fatty acids as well as different levels of impurities in the feedstock. Polymerisations were carried out in toluene using AIBN as an initiator and DDMAT was selected as an appropriate chain transfer agent. <sup>1</sup>H NMR spectroscopy and GPC were used to obtain monomer conversion, M<sub>w</sub> and Đ kinetics data from the polymerisations that was subsequently used to assess the control of the reaction by the RAFT agent.

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