EaStCHEM Workshop on Sustainable Synthesis for Net Zero

(Theatre B, School of Chemistry, University of St. Andrews, August 31, 2023)

09:30-09:50 Coffee
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09:50 - 10:00 Welcome/acknowledgements by Dr. Amit Kumar

Session 1. Chair: Dr. Jennifer Garden, University of Edinburgh
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10:00 - 10:40 Prof. David Cole-Hamilton (Chemicals from waste bio-oil towards commercialisation)

10:40 - 11:20 Dr. Thomas Schaub (Industrially relevant organic synthesis using CO_2 and CO_2 related processes @BASF @CaRLa

11:20 – 12:00 Dr. Paul Price, Unilever (Sustainability Innovations for a Planet Positive Fast Moving Consumer Goods Industry)

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12:00 - 13:30. Lunch
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Session 2. Chair: Prof. David O'Hagan, University of St. Andrews
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13:30 - 14:10 Prof. Stephen Wallace (Bio-H2 for Sustainable Alkene Hydrogenation using Living Bacteria)

14:10 - 14:50 Dr. Amanda Jarvis (A journey in sustainable catalysis: from homogeneous catalysis to artificial enzymes)

14:50 - 15:30 Dr. Claire Brodie (Renewable polymers and a case study of polyethyleneimines)
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15:30 - 16:00. Coffee
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Session 3. Chair: Prof. Andrew Smith, University of St. Andrews
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16:00 - 16:40 Dr. Paul Webb (Connecting a future energy system with carbon recycle for chemicals production)

16:40 -17:20 Dr. Matthew Brander (Introduction to Life Cycle Assessment (LCA))

17:20 – 18:00 Dr. Thomas Schaub (Case studies of carbon-footprint in research projects (Formaldehyde & sodium acrylate from CO2) @BASF and LCA

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Prof. David Cole-Hamilton

Biography

David Cole-Hamilton obtained his BSc and PhD at Edinburgh University, before working with Sir Geoffrey Wilkinson at Imperial College. He was Lecturer and Senior Lecturer at Liverpool University before moving to be Professor of Chemistry at the University of St. Andrews in. He became Emeritus in 2014.

He was President of the European Chemical Society (2013-7) and has won a number of prizes from the Royal Society of Chemistry as well as 5 prizes for teaching. In 2017 he was awarded the Alwin Mittasch Prize of the German Catalysis Society and was made a Foreign Member of the Russian Academy of Natural Sciences but resigned in 2022 in protest at the Russian invasion of Ukraine.

He worked on the production of useful chemicals from waste bio-oils to replace oil derived compounds. He is currently trying to scale up some of these routes for commercialisation.

Abstract

Chemicals from waste bio-oils towards commercialisation

David J. Cole-Hamilton,[a]*Philip Kenyon[a], Paul Webb[a], Ronan le Goff,[a] Marc Furst,[a] Juma Mmongoyo,[a,b] James Mgaya,[a,b] Jennifer Julis,[a] Stuart Bartlett,[a] Sabrina Baader,[c] Yiping Shi[a] and Quintino Mgani[b]

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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 but being aware of land use.

We shall show how homogeneous carbonylation,[1] metathesis, and reductive amination[2] can be used to make difunctional esters acids, alcohols, amines[1, 3-5] for polymer formation from unpurified natural oils containing oleate residues

Cashew nut shell liquid contains interesting phenols *meta* substituted with an unsaturated C_{15} chain. We shall described how it can be used to synthesise compounds that can be used in a range of different applications.[6-9]

We shall discuss the features that may make it possible to commercilaise some of these desirable molecules but not others and our moves towards setting up a biorefinery..

References

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9. Y. P. Shi, P. C. J. Kamer and D. J. Cole-Hamilton, *Green Chemistry*, 2019, **21**, 1043-1053.

Dr. Thomas Schaub

Biography
Born in 1980 in Lahr/Black Forest
1999-2002 Undergraduate studies in Chemistry at the University of Karlsruhe (TH)
2002-2004 Graduate Studies, Diploma in Chemistry and Diploma-Thesis with Dr. U. Radius, Institute of Inorganic Chemistry, University of Karlsruhe (TH)
2004-2006 PhD and Dissertation with Dr. U. Radius, Institute of Inorganic Chemistry, University of Karlsruhe (TH)
2007-2008 Postdoctoral Fellow in the Group of Prof. Dr. D. Milstein, Department of Organic Chemistry, Weizmann Institute of Science, Israel
2008-2014 Research Scientist in the group for homogeneous catalysis development within the Process Research and Chemical Engineering Unit ("Ammonlabor") at BASF SE in Ludwigshafen
Since 2014 Lab Head of the Catalysis Research Laboratory (CaRLa) in Heidelberg
Since 2018 Designated Principal Scientist for Homogeneous Catalysis
Since 2022 Honorary Professor at the University of St. Andrews
www.st-andrews.ac.uk/chemistry/people/ts298/
Awards and Fellowships
2002-2004 Fellow of the Fritz-ter-Mer foundation (Leverkusen)
2007-2008 Feodor Lynen Research Fellowship of the Minerva foundation (Munich)
Research Interests
• Process Development using homogeneous catalysis on: Hydrogenations, Aminations, Acceptorless Dehydrogenations, Oligomerisations, Carbonylations
• Use of CO2 as building block
• Efficient use of renewables as building blocks in organic synthesis
• ChemCycling
• Organometallic Synthesis
• Mechanistic investigations on homogeneous catalyzed reactions
• High pressure chemistry
Co-author of 68 scientific publications (thereof as 52 as reference author), three book chapters and Co-inventor on 82 patent applications, Invited Speaker on different conferences and holding lectures at several universities.

Abstract

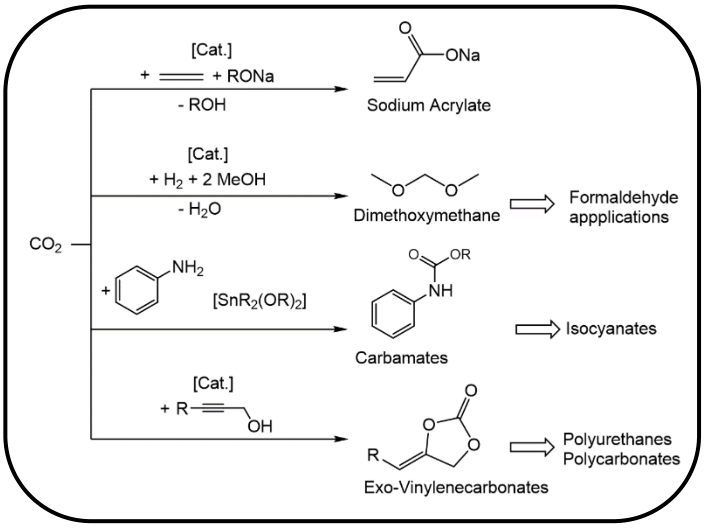
Part 1: Industrially relevant organic synthesis using CO_2 and CO_2 related processes @BASF/CaRLa

Prof. Dr. Thomas Schaub, BASF/CaRLa; thomas.schaub@basf.com; www.carla-hd.de

CO_2 is an abundant and cheap carbon building block and therefore of high interest.[1] But as CO_2 is the energetically final product of the combustion of organic materials, irrespective of which organic product one wants to make out of CO_2, the reaction needs a driving force by a energetic reaction partner and/or energy input to the process. If a dedicated use of CO_2 as a building block has the potential to reduce greenhouse potential therefore strongly depends on the greenhouse potential/carbon footprint of the driving force. Additionally, from an industrial view, it must be economically viable.

In the first part of this talk, an overview will be given on the processes already used in industry utilizing CO_2 and on different projects @CaRLa on the developed of new processes for BASF utilizing CO_2:

- Sodium acrylate based on CO_2[2]
- Formaldehyde from CO_2[3]
- Isocyanates based on CO_2[4]
- Exo-Vinylenecarbonates[5]



In the second part, two more detailed and critical case studies on the carbon footprint evaluation/LCA of the two processes fromaldehyde and sodium acrylate based on CO_2 will be given.

References:
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Dr. Paul Price

Biography

Paul Price is a Science & Technology Programme Leader for renewable ingredient development, and a Team Leader in Unilever R&D, supporting the Beauty & Wellbeing and Personal Care business groups. In a fifteen year career, Paul has worked on a range of technologies across Unilever's home and personal care portfolio. Prior to joining Unilever, Paul spent three years working on novel therapeutics to treat neuromuscular diseases at Summit plc, a spin out from the University of Oxford. Prior to this Paul studied for an MChem and DPhil in chemistry from the University of Oxford, the latter under the supervision of Prof Steve Davies, where he developed novel routes for the asymmetric synthesis of azasugars via lithium amide addition chemistry.

Abstract

Sustainability Innovations for a Planet Positive Fast Moving Consumer Goods Industry

The fast moving consumer goods (FMCG) industry generates significant value globally and delivers products which meet the fundamental needs of consumers across all income levels around the world. Unilever is a major player in the Personal Care, Beauty and Home Care sectors. The sheer size of these markets globally means that companies operating in this space have an opportunity to use their scale for good, and must look to grow in a way that positively impacts people and planet. Delivering a future net zero FMCG industry will require changes across the whole value chain, with companies addressing emissions from within their direct operations and extended value chains. Technological innovations will provide routes to ingredients and products with very low carbon footprints, but significant challenges still exist to ensure these nascent value chains can deliver ingredients at the scale and cost needed for use in consumer goods.

Prof. Stephen Wallace

Biography

Professor Stephen Wallace is a UKRI Future Leaders Fellow and Chair of Chemical Biotechnology in the School of Biological Sciences at the University of Edinburgh.

He has a MChem in Medicinal and Biological Chemistry from the University of Edinburgh and a DPhil in Organic Chemistry from the University of Oxford. He has held postdoctoral Fellowships at the MRC Laboratory of Molecular Biology in Cambridge (with Prof. Jason Chin), the Department of Chemistry and Chemical Biology at Harvard University (with Prof. Emily Balskus) and the Department of Chemistry at the University of Cambridge (with Prof. Steve Ley). In 2019, he was a visiting Professor at the Rosen Centre for Bioengineering at Caltech (with Prof. Frances Arnold).

He began his independent career at the University of Edinburgh in 2017 as a Lecturer in Biotechnology, where he was promoted to Senior Lecturer in 2020, and Professor of Chemical Biotechnology in 2023.

Current projects in his lab include the use of unexplored microorganisms for chemical synthesis, the construction of new biosynthetic pathways in bacteria, the evolution of new enzymatic function, and the valorisation of waste materials into fine chemicals using biocompatible chemistry.

Abstract:

Bio-H2 for Sustainable Alkene Hydrogenation using Living Bacteria

Hydrogenation is one of the most ubiquitous reactions used in chemical industry. It has been estimated that 25% of all clinical drug candidates contain at least one hydrogenation step in their synthetic sequence. However, nearly all H2 used in industry is generated from fossil fuels via steam reforming, despite the fact that H2 is a metabolite in Nature and therefore can be produced via metabolic engineering from sustainable resources. In my talk I will present our most recent research into the use of bacterial hydrogen gas for non-enzymatic alkene and metabolite hydrogenation using biocompatible Pd catalysis in vivo. Overall, this work demonstrates how biocompatible non-enzymatic reactions can be interfaced with engineered microbial metabolism to enable synthetic transformations that cannot be achieved using enzymatic chemistry alone.

Dr. Amanda Jarvis

Biography
Amanda graduated from the University of St. Andrews (UK) in 2007 with a Masters in Chemistry. Following her undergraduate studies, she went on to receive a PhD from the University of York (UK) under the supervision of Professor Ian Fairlamb. Amanda joined the group of Dr Philippe Dauban (ICSN, Gif-sur-Yvette) as a postdoctoral research fellow in 2011 and worked on the development of Rh(II)-catalysed nitrene reactions. In 2013, she moved to Professor Paul Kamer group to work on the development of Artificial Metalloenzymes. In 2015, she received a Marie Curie Individual Fellowship to continue working in Prof. Paul Kamer's group on Artificial Metalloenzymes for the Oxidation of Alkanes (ArtOxiZymes). In October 2017, Amanda started her independent career at the University of Edinburgh as a Christina Miller Fellow, and was awarded a UKRI Future Leaders Fellowship in May 2019. In 2022, she was promoted to Senior Lecturer.

Abstract

A journey in sustainable catalysis: from homogeneous catalysis to artificial enzymes

I will discuss my personal journey from homogeneous catalysis to setting up a research group working on artificial enzymes. I will use examples from our work to illustrate how sustainability has been a common thread throughout my research career. I will highlight how my group combines biology and chemistry to address current issues facing the chemical community in light of its bid to reach net zero.

Dr. Claire Brodie

Biography

Dr Claire Brodie did her undergraduate studies here at the University of St Andrews before moving to Durham for a PhD under the supervision of Professor Phil Dyer where she worked on cobalt complex synthesis and reactivity for olefin oligomerisation. After this, she joined the group of Professor Andrew Weller in a postdoctoral role where she developed group 9 systems for amine-borane dehydropolymerisation and polyaminoborane depolymerisation. In 2022, Claire returned to Scotland and the University of St Andrews to continue postdoctoral work in the group of Dr Amit Kumar where she works on developing green syntheses for polymerisation and depolymerisation reactions using homogeneous catalysis.

Abstract

The manganese catalysed dehydrative coupling of amines and alcohols to polyethyleneimine

Claire N. Brodie, Aniekan E. Owen, Micheal Bühl and Amit Kumar
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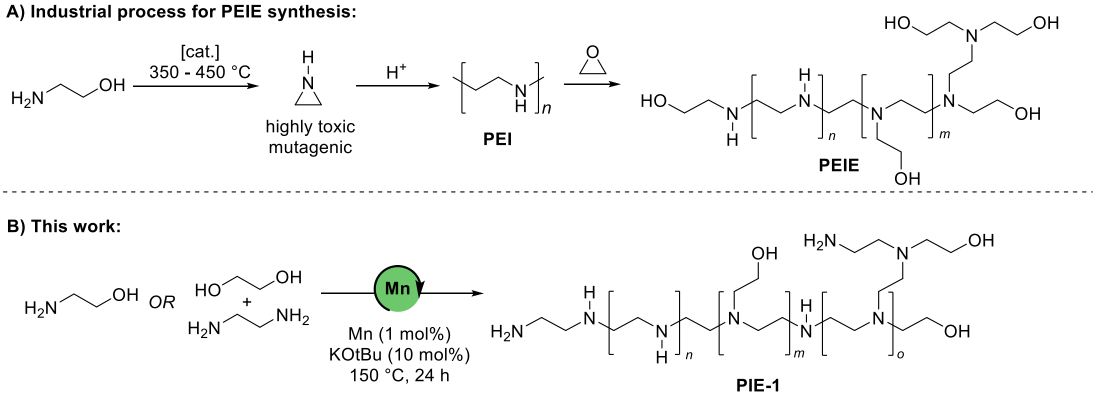
Polyethylene imine (PIE) and derivative, polyethyleneimine ethoxylated (PEIE) are industrially relevant polymers that are widely applied in detergents, adhesives, cosmetics, and water treatment and gene-delivery agents.[1,2] Currently, PEI is produced from a highly toxic, mutagenic and volatile compound, aziridine (C_2H_5N), which is, in turn, prepared from dehydration of aminoethanol under energy intensive conditions, and PEIE is prepared from reaction of PEI with ethylene oxide (Scheme 1A). Here, we report[3,4] a sustainable route for the preparation of a new polymer, PEI-1 (Scheme 1B) with similar properties to PEIE from renewable feedstocks, such as ethylene glycol and ethylene diamine, mediated through application of the Earth-abundant Mn-MACHO (MACHO = (*N*,*N*-*bis*{di*iso*propylphosphinoethyl}amine)) precatalyst. The reaction allows for the selective generation of PEI-1 as high molecular weight (M_n > 40,000 g mol^{-1}) material in >90% isolated yield under, relatively, mild conditions. The intrinsic thermal and physical properties of the polymeric product are investigated and reported. The method of polymerisation is investigated through dual experimental (e.g. stochiometric experiments, kinetics of polymerisation, gas evolution, etc.) and computational approaches and a mechanism of polymerisation proposed.



Scheme 1 Methodology for the preparation of ethoxylated polyethyleneimines.

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Dr. Paul Webb

Biography

Paul Webb obtained his BSc and PhD at The University of Nottingham, before working with David Cole-Hamilton at the University of St Andrews. He then moved to the global petrochemical company Sasol, where he was employed as Chief Scientist for 13 years. He led a team of experienced scientists charged with the task of understanding structure-performance relationships in catalysis and the translation of fundamental research into commercial benefit. In his final years at Sasol he held a Royal Society Industry Fellowship jointly with the University of St Andrews, a position that ultimately led to his transition back to academia in 2019. Over the past 20 years he has worked extensively at the interface between industry and academia, turning discovery phase research into commercial technology. His current research interests lie in the development of sustainable processes with particular emphasis on Power-to-X concepts.

Lecture Title: Connecting a future energy system with carbon recycle for chemicals production

Dr. Mathew Brander

Biography

Matthew is a Senior Lecturer in Carbon Accounting at the University of Edinburgh's Business School. His current research focuses on the development of methods for corporate, product (life cycle assessment), project and policy-level greenhouse gas accounting. He has particular interest in bioenergy, offsetting, electricity accounting, greenhouse gas removal, and the alignment of financial flows with the Paris Agreement. He has served as a member of several technical working groups for the Greenhouse Gas Protocol, and the International Organisation for Standardisation (ISO), and is on the peer review panel for Department for Energy Security and Net Zero's (DESNZ) emission factors publication for company reporting, and the Advisory Board for the Woodland Carbon Code. He also chairs the Climate Advisory Group for abrdn's Multi-Asset Climate Solutions Fund. Prior to his current position Matthew worked for over seven years in carbon management and greenhouse gas assessment at the Edinburgh Centre for Carbon Management, and at Ecometrica. For more information: https://www.business-school.ed.ac.uk/staff/matthew-brander

Abstract

Introduction to Life Cycle Assessment

Life cycle assessment (LCA) is a widely used analytical method for quantifying the environmental (and sometimes social) impacts of products, technologies, materials etc. One of the underpinning rationales for studying the whole life cycle is to avoid reducing impacts at one life cycle stage, but inadvertently increasing impacts at other life cycle stages. The most widely used form of LCA is 'attributional' LCA, which aims to quantify all the material and energy flows from processes used within the life cycle, and the associated impacts. However, ALCA does not reflect the total system-wide change in impacts caused by a product as it does not include market-mediated effects. Consequential LCA aims to quantify system-wide change and is therefore arguably the appropriate method for informing decisions, given that decisions should be made based on their consequences. However, even CLCA has limitations, and emerging methods such as 'baseline-and-intervention assessment' provide additional information on the timing of impacts.